STIC Search Report
Biotech-Chem Library

STIC Database Tracking Number: 163499

TO: Shobha Kantamneni **Location: 4c29 / 4b18** **Wednesday, August 24, 2005** **Art Unit: 1617** **Phone: 571-272-2930** **Serial Number: 09 / 893861**	**From: Jan Delaval** **Location: Biotech-Chem Library** **Remsen 1a51** **Phone: 571-272-2504** **jan.delaval@uspto.gov**

Search Notes

```
=> fil reg
FILE 'REGISTRY' ENTERED AT 08:08:57 ON 24 AUG 2005
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:   22 AUG 2005  HIGHEST RN 861291-85-2
DICTIONARY FILE UPDATES:  22 AUG 2005  HIGHEST RN 861291-85-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from     *
* the IDE default display format and the ED field has been added,       *
* effective March 20, 2005.  A new display format, IDERL, is now        *
* available and contains the CA role and document type information.     *
*                                                                       *
*************************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que l21
L13                 STR
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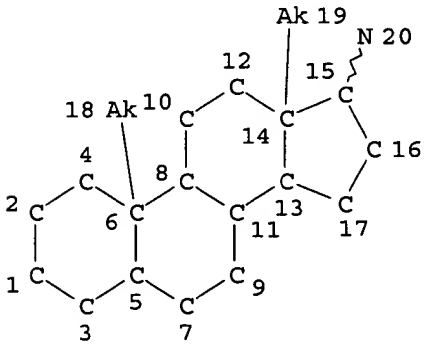


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NODE ATTRIBUTES:
CONNECT IS M1  RC AT   1
CONNECT IS M1  RC AT  20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
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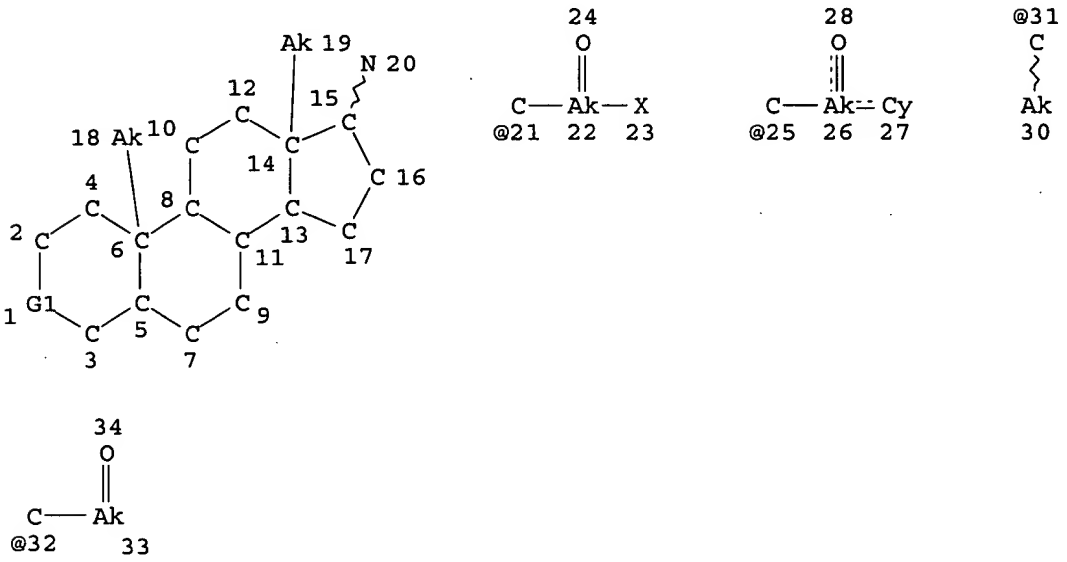
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L15 758 SEA FILE=REGISTRY CSS FUL L13
L19 STR



VAR G1=C/32/21/25/31
NODE ATTRIBUTES:
CONNECT IS M1 RC AT 20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC 1
NUMBER OF NODES IS 33

STEREO ATTRIBUTES: NONE
L21 93 SEA FILE=REGISTRY SUB=L15 CSS FUL L19

100.0% PROCESSED 758 ITERATIONS 93 ANSWERS
SEARCH TIME: 00.00.01

=> d his

(FILE 'HCAPLUS' ENTERED AT 07:46:04 ON 24 AUG 2005)
DEL HIS
L1 1 S US20030216361/PN OR (US2001-893861# OR US2000-214844#)/AP,PRN
E PETTIT G/AU
L2 73 S E3,E9,E10
L3 696 S E14-E16,E21-E24
L4 1 S E26
L5 162 S E112,E118,E135,E136
SEL RN L1

FILE 'REGISTRY' ENTERED AT 07:48:03 ON 24 AUG 2005
L6 5 S E1-E5
L7 1 S L6 AND C5-C6-C6-C6/ES AND N/ELS

```
                E C26H42N2O3/MF
L8              1 S E3 AND C5-C6-C6-C6/ES AND NC4/ES
L9              1 S 13574-69-1/CRN
L10             2 S L7-L9
                E 4432.3/RID
L11         83023 S E4
L12         29539 S L11 AND N/ELS
L13               STR
L14            30 S L13 CSS
L15           758 S L13 CSS FUL
                  SAV L15 KANTAM893/A
L16               STR L13
L17             0 S L16 CSS SAM SUB=L15
L18             0 S L15 AND SQL/FA
L19               STR L16
L20             2 S L19 CSS SAM SUB=L15
L21            93 S L19 CSS FUL SUB=L15
                  SAV L21 KANTAM893A/A
L22             7 S L21 AND C19H33N
L23             9 S L10,L22
                  SAV L23 KANTAM893B/A

     FILE 'HCAOLD' ENTERED AT 08:03:20 ON 24 AUG 2005
L24             2 S L23
                  SEL AN
                  EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 08:04:21 ON 24 AUG 2005
L25             4 S E1-E2
L26             2 S L25 NOT (METHYLESTRADIOL OR ERGOSTEROL)/TI
L27            13 S L23
L28             2 S L26 AND L27
L29            11 S L27 NOT L28
L30             3 S L29 AND L1-L5
L31            12 S L27 AND (PD<=20000628 OR PRD<=20000628 OR AD<=20000628)
L32            11 S L26-L31 NOT L28
L33             2 S (3 BETA OR 3BETA OR 3B OR E B)()ACETOXY()(17BETA OR 17B OR 17
L34            11 S L32,L33

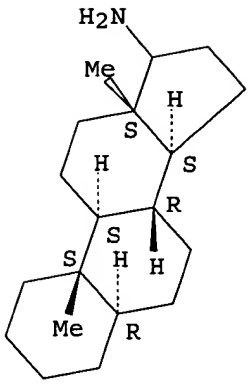
     FILE 'USPATFULL' ENTERED AT 08:08:28 ON 24 AUG 2005
L35             9 S L23

     FILE 'REGISTRY' ENTERED AT 08:08:57 ON 24 AUG 2005

=> d ide can tot l23

L23  ANSWER 1 OF 9  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   757123-55-0  REGISTRY
ED   Entered STN:  05 Oct 2004
CN   Androstan-17-amine, (5α)- (9CI)  (CA INDEX NAME)
FS   STEREOSEARCH
MF   C19 H33 N
CI   COM
SR   CA

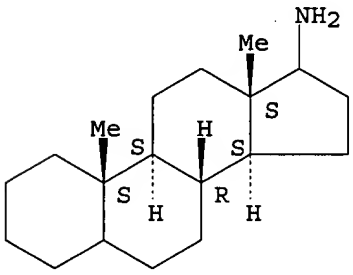
Absolute stereochemistry.
```



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L23 ANSWER 2 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 496858-17-4 REGISTRY
ED Entered STN: 04 Mar 2003
CN Androstan-17-amine (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF **C19 H33 N**
SR Chemical Library
Supplier: Interchim

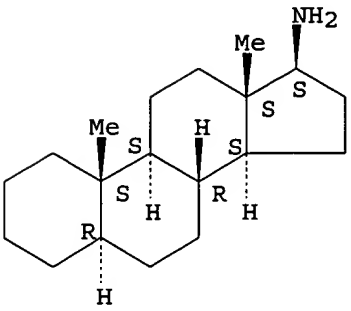
Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L23 ANSWER 3 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 54156-37-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Androstan-17-amine, hydrochloride, (5α,17β)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17β-Amino-5α-androstane hydrochloride
FS STEREOSEARCH
MF **C19 H33 N . Cl H**
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)
CRN (31239-17-5)

Absolute stereochemistry.



● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

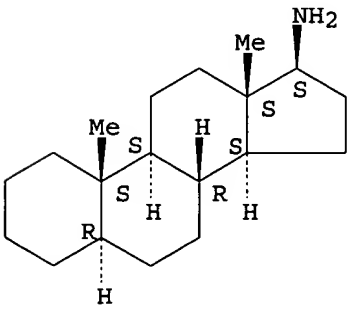
REFERENCE 1: 81:152498

L23 ANSWER 4 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 54156-36-4 REGISTRY
ED Entered STN: 16 Nov 1984
CN Androstan-17-amine, (5α,17β)-, acetate (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 17β-Amino-5α-androstane acetate
FS STEREOSEARCH
MF **C19 H33 N . C2 H4 O2**
LC STN Files: CA, CAPLUS

CM 1

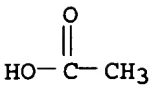
CRN 31239-17-5
CMF C19 H33 N

Absolute stereochemistry.



CM 2

CRN 64-19-7
CMF C2 H4 O2

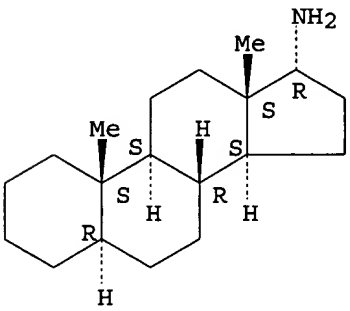


1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 81:152498

L23 ANSWER 5 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 31239-23-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5α-Androstan-17α-amine (8CI)
FS STEREOSEARCH
MF **C19 H33 N**
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

5 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 81:152498

REFERENCE 2: 75:128415

REFERENCE 3: 74:125901

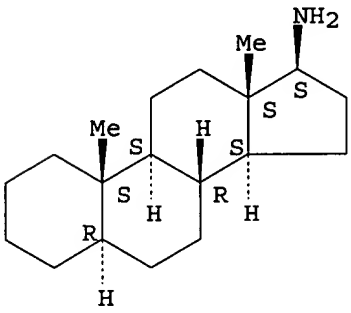
REFERENCE 4: 74:88205

REFERENCE 5: 56:53616

L23 ANSWER 6 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 31239-17-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5α-Androstan-17β-amine (6CI, 7CI, 8CI)

OTHER NAMES:
CN 17β-Amino-5α-androstane
FS STEREOSEARCH
MF **C19 H33 N**
CI COM
LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

8 REFERENCES IN FILE CA (1907 TO DATE)
8 REFERENCES IN FILE CAPLUS (1907 TO DATE)
2 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 141:350323

REFERENCE 2: 117:90139

REFERENCE 3: 108:75714

REFERENCE 4: 92:181459

REFERENCE 5: 81:152498

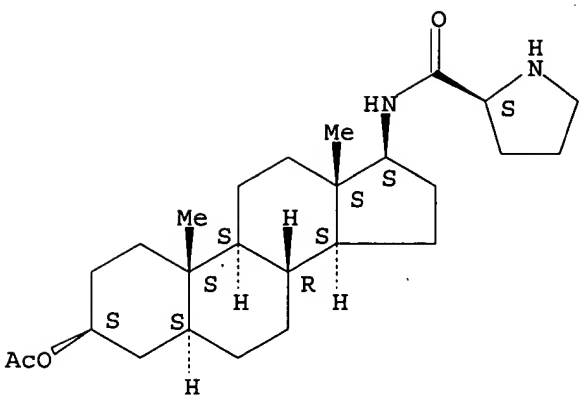
REFERENCE 6: 74:125901

REFERENCE 7: 74:88205

REFERENCE 8: 53:67855

L23 ANSWER 7 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 13574-72-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Pyrrolidinecarboxamide, N-(3β-hydroxy-5α-androstan-17β-yl)-, acetate (ester), monohydrochloride, L- (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5-α-Androstan-3β-ol, 17β-(L-2-pyrrolidinecarboxamido)-, acetate (ester), monohydrochloride
FS STEREOSEARCH
MF C26 H42 N2 O3 . Cl H
LC STN Files: CA, CAPLUS
CRN (13574-69-1)

Absolute stereochemistry.



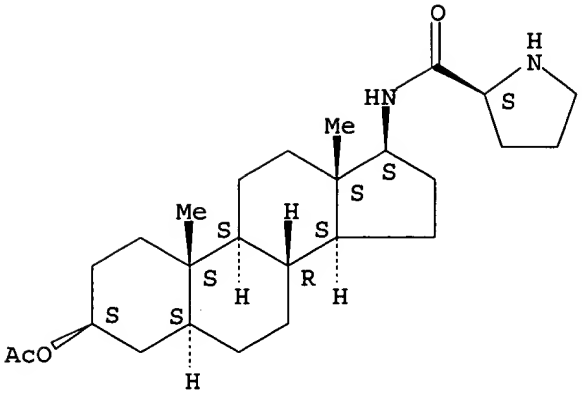
● HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

L23 ANSWER 8 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN **13574-69-1** REGISTRY
ED Entered STN: 16 Nov 1984
CN 2-Pyrrolidinecarboxamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, (2S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pyrrolidinecarboxamide, N-(3β-hydroxy-5α-androstan-17β-yl)-, acetate (ester), L- (8CI)
CN 5α-Androstan-3β-ol, 17β-(L-2-pyrrolidinecarboxamido)-, acetate (ester)
FS STEREOSEARCH
MF **C26 H42 N2 O3**
CI COM
LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER, USPATFULL
(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

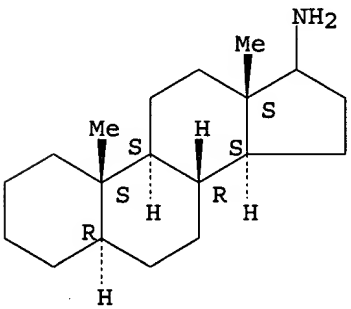
REFERENCE 1: 139:374985

REFERENCE 2: 133:203156

REFERENCE 3: 66:76285

L23 ANSWER 9 OF 9 REGISTRY COPYRIGHT 2005 ACS on STN
RN 5953-55-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Androstan-17-amine, hydrochloride, (5α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5α-Androstan-17β-amine, hydrochloride (7CI, 8CI)
FS STEREOSEARCH
MF **C19 H33 N . Cl H**
LC STN Files: BEILSTEIN*, CAOLD
(*File contains numerically searchable property data)
CRN (757123-55-0)

Absolute stereochemistry.



● HCl

1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

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FILE 'HCAOLD' ENTERED AT 08:09:14 ON 24 AUG 2005

PRE-1967 CHEMICAL ABSTRACTS FILE WITH HOUR-BASED PRICING
FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

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This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

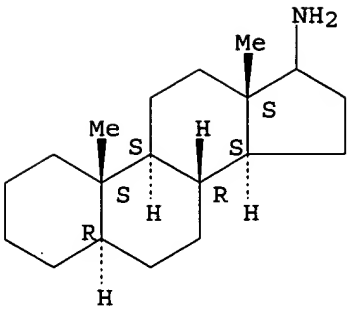
=> d all hitstr tot l24

L24 ANSWER 1 OF 2 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA56:10233h CAOLD
TI 17-aminoandrostanes
AU Babcock, John C.
PA Upjohn Co.
DT Patent

PATENT NO.	KIND	DATE
US 3009925		1961
DE 1165023		
GB 916138		

IT 1474-16-4 1818-11-7 2354-27-0 2966-91-8 3240-39-9 5668-07-5
5953-55-9 31239-17-5 54498-44-1 94763-52-7
94763-58-3 94969-71-8 95135-26-5 95191-12-1 95340-36-6 95367-61-6
95367-67-2 95462-27-4 95462-28-5 100433-88-3 100468-80-2
IT **5953-55-9 31239-17-5**
RN 5953-55-9 HCAOLD
CN Androstan-17-amine, hydrochloride, (5α)- (9CI) (CA INDEX NAME)

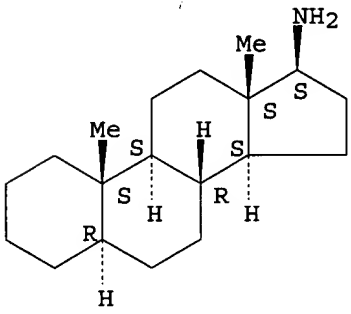
Absolute stereochemistry.



● HCl

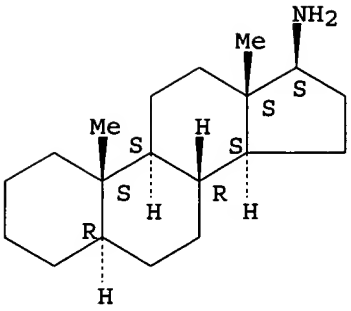
RN 31239-17-5 HCAOLD
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L24 ANSWER 2 OF 2 HCAOLD COPYRIGHT 2005 ACS on STN
AN CA53:12345b CAOLD
TI steroids and Walden inversion - (XLI) deamination of A-nor-, B-nor-, and 17-aminosteroids
AU Shoppee, Charles W.; Sly, J. C. P.
IT 1178-00-3 2310-36-3 2311-96-8 2493-92-7 4350-66-7 4350-67-8
6908-01-6 14772-37-3 14772-59-9 20853-64-9 28097-22-5 29599-03-9
31239-17-5 35878-83-2 56997-89-8 70182-75-1 85198-44-3
103366-02-5 110346-39-9 119677-75-7 122386-63-4 122386-64-5 122386-65-6
122386-75-8 122386-76-9 122386-85-0 122386-90-7 122441-37-6 122441-42-3
122564-84-5 122626-62-4 122650-16-2 122650-17-3 122650-18-4
IT **31239-17-5**
RN 31239-17-5 HCAOLD
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.




```
=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:09:29 ON 24 AUG 2005
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FILE COVERS 1907 - 24 Aug 2005  VOL 143 ISS 9
FILE LAST UPDATED: 22 Aug 2005  (20050822/ED)

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 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

=> => d all tot hitstr l28

L28  ANSWER 1 OF 2  HCAPLUS  COPYRIGHT 2005 ACS on STN
AN   1962:53616  HCAPLUS
DN   56:53616
OREF 56:10233h-i,10234a-g
ED   Entered STN:  22 Apr 2001
TI   17-Aminoandrostanes
IN   Babcock, John C.
PA   Upjohn Co.
DT   Patent
LA   Unavailable
CC   36 (Steroids)
FAN.CNT 1
     PATENT NO.          KIND   DATE      APPLICATION NO.         DATE
     ---------------     ----   --------  --------------------    --------
PI   US 3009925                 19611121  US                      19591207
     DE 1165023                           DE
     GB 916138                            GB
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PRAI US 19591207

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 3009925	NCL	552/522.000; 424/115.000; 552/516.000; 552/519.000; 552/577.000; 552/610.000; 552/611.000; 552/641.000

AB 17-Isonitroso-5α-androstan-11β-ol(20 g.) in 180 ml. iso-PrOH and 180 ml. Et2O stirred 3 hrs. with 20 g. Li in 1.5 l. liquid NH3, treated with 40 ml. iso-PrOH, evaporated, the residue washed, treated with 40 ml. 2.5N HCl, and crystallized gave 10.2 g. 17β-amino-5α-androstan-11β-ol-HCl (I), m. 300-4° (decomposition). I (5.55 g.) in 55 ml. 10% aqueous KOH and 200 ml. Et2O stirred, separated, evaporated, and crystallized gave 17β-amino-5α-androstan-11β-ol (II), m. 192-3°. The ether solution of the reduction product remaining after the HCl salt bad been precipitated, washed, and evaporated gave 10.55 g. 17αamino-5α-androstan-11β-ol (III), m. 91-100° (decomposition). III treated with dry HCl gave the HCl salt, m. 161.5-5.0° (decomposition). II (6 g.) in 60 ml. C5H5N left several hrs. with 12 ml. Et chlorocarbonate gave the N-carbethoxy derivative (IV), purified by chromatography. IV oxidized with CrO3 and AcOH gave 17β-amino-5α-androstan-11-one N-carbethoxy derivative (V). V hydrolyzed with 10-20% NaOH in (CH2OH)2 gave 17β-amino-5α-androstan-11-one. II (5.22 g.) in 4.2 ml. HCO2H and 3.6 ml. HCHO warmed 1.5 hrs. at 80°, cooled, evaporated, the residue taken up in CH2Cl2, washed, and evaporated gave 1.8 g. 17β-dimethylamino-5αandrostan-11β-ol (VI), m. 161.5-3.0° HCl salt prepared via HCl gas. VI (1.86 g.) treated 15 hrs. with 5 ml. MeI gave 1.06 g. 17β-dimethylamino-5α-androstan-11β-ol-MeI, m. 307-8°. Following this procedure 17β-diethylamino-5αandrostan-11β-ol was prepared by use of AcH. The HCl and MeI salts were prepared 9α-Fluoro-17-isonitroso-5α-androstan-11β-ol (VII) was prepared from 9(11)-androsten-17-one by reaction with N-bromoacetamide in aqueous HClO4 and the 9αbromo-11β-hydroxy-5α-androstan-17-one so formed treated with KOAc in alc. gave first 9β,11β-oxido-5α-androstan-17-one, which with anhydrous HF gave 9α-fluoro-11β-hydroxyandrostan-17-one (VIII). VIII oxidized with CrO3 in AcOH gave 9α-fluoroandrostane-11,17-dione (IX). VIII and IX were converted with NH2OH.HCl in C5H5N to VII and 9β-fluoro-17-isonitroso-5α-androstan-11-one, resp. These two compds. reduced catalytically gave 17β-amino-9α-fluoro-5α-androstan-11β-ol (X) and 17β-amino-9α-fluoro-5α-androstan-11-one, resp. X was converted into 17β-dimethylamino-9α-fluoro-5α-androstan-11β-ol, HCl salt, and MeI salt. II (6 g.) in 60 ml. C5H5N left 2 hrs. with 12 ml. ClCO2Et gave the amorphous urethan, purified by chromatography on Florisil. This urethan in 200 ml. tetrahydrofuran refluxed 15 hrs. with 6 g. LiAlH4 in the same solvent, decomposed, treated with 12 ml. 20% KOH and 12 ml. H2O, filtered, and the filtrate evaporated gave HCl salt of 17β-methylamino-5α-androstane, m 307-10° (MeOH-2.5N HCl). II (5.3 g.) in 4.6 ml. HCO2H and 4 ml. HCHO warmed 1 hr. with effervescence, then refluxed 1.5 hrs., evaporated, the residue taken up in Et2O and CH2Cl2, and the product recrystd. gave 2.7 g. 17β-dimethylamino-5α-androstane (XI), m. 87-98.5°; HCl salt m. 281-2°. II with ClCO2Et gave 17β-amino-5α-androstan-11β-ol N-carbethoxy derivative and this product reduced with LiAlH4 gave 17β-methylamino-5α-androstan-11β-ol. The sulfates and phosphates of the above compds. were readily prepared XI (0.7 g.) in 25 ml. alc. and 5 ml. MeI left 18 hrs. and poured into Et2O gave 17β-dimethylamino-5α-androstane-MeI, m. 281.5-3.5° (decomposition). 17-Isonitroso-9(1'1)-androstene was converted to

17β-amino-9(11)-androstene-HCl and then into 17β-amino-9(11)-androstene. X afforded 17β-methylamino-9α-fluoro-5α-androstan-11β-ol. 17-Isonitroso-5αandrostan-11α-ol gave 17-amino-5α-androstan-11α-ol-HCl. Typical compns. embodying the above compds. for pharmacol. use were described.

IT Fungicides or Fungistats
(5α-androstan-17β-amine and derivs. as)

IT Androgenic hormones or principles
(inhibitors, 2-methylestra-1,3,5(10)-triene-3,17β-diol as)

IT 5α-Androstan-11α-ol, 17β-amino-
5α-Androstan-11α-ol, 17β-amino-, hydrochloride
5α-Androstan-11β-ol, 17α-amino-, hydrochloride
5α-Androstan-11β-ol, 17β-(dimethylamino)-, methiodide
5α-Androstan-17α-amine, hydrochloride
5α-Androstan-17α-amine, N,N-dimethyl-
5α-Androstan-17α-amine, N,N-dimethyl-, hydrochloride
5α-Androstan-17α-amine, N,N-dimethyl-, methiodide
5α-Androstan-17α-amine, N-methyl-, hydrochloride
Ammonium, (11β-hydroxy-5α-androstan-17β-yl)trimethyl, iodide
Ammonium, (5α-androstan-17β-yl)trimethyl, iodide

IT 438-22-2, Androstane
(11,18-dioxygenated derivs.)

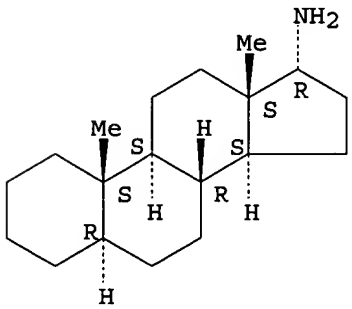
IT 1474-16-4, 5α-Androstan-11β-ol, 17β-amino-, hydrochloride
2354-27-0, 5α-Androstan-11β-ol, 17β-amino-9-fluoro-
2966-91-8, 5α-Androstan-11β-ol, 17β-amino-9-fluoro-, hydrochloride 5668-07-5, 5α-Androstan-11β-ol, 17β-amino-
31239-23-3, 5α-Androstan-17α-amine 61148-15-0,
5α-Androstan-11β-ol, 17α-amino- 94763-58-3,
5α-Androstan-11β-ol, 17β-(methylamino)- 94969-71-8,
5α-Androst-9(11)-en-17β-amine, N,N-dimethyl- 95135-26-5,
5β-Androstan-11β-ol, 17β-(dimethylamino)-, hydrochloride
95340-36-6, 5β-Androstan-11β-ol, 17β-(dimethylamino)-
95367-61-6, 5α-Androst-9(11)-en-17β-amine, hydrochloride
95367-67-2, 5α-Androstan-11-one, 17β-amino-, hydrochloride
95462-27-4, 5α-Androst-9(11)-en-17β-amine 95462-28-5,
5α-Androstan-11-one, 17β-amino-
(preparation of)

IT **31239-23-3**, 5α-Androstan-17α-amine
(preparation of)

RN 31239-23-3 HCAPLUS

CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1959:67855 HCAPLUS
DN 53:67855
OREF 53:**12345b-i,12346a-h**
ED Entered STN: 22 Apr 2001
TI Steroids and Walden inversion. XLI. Deamination of some A-nor-, B-nor-, and 17-aminosteroids
AU Shoppee, C. W.; Sly, J. C. P.
CS Univ. Coll., Swansea, S. E. Wales
SO Journal of the Chemical Society, Abstracts (1959) 345-56
CODEN: JCSAAZ; ISSN: 0590-9791
DT Journal
LA Unavailable
CC 10J (Organic Chemistry: Steroids)
OS CASREACT 53:67855
AB cf. C.A. 53, 1412g. NH2 groups attached to flexible 5-membered carbocyclic systems, e.g., cyclopentane, cis-perhydroindan, appear to possess mixed equatorial-axial character. NH2 groups attached to rigid 5-membered carbocyclic systems, e.g. trans-perhydroindan, or to such systems forming part of the nuclei of A-nor-5α-, A-nor-5β- and 14α-steroids, at positions adjacent to a bridgehead, appear to possess either equatorial character disclosed by deamination with retention of configuration, or axial character disclosed by deamination with ready and exclusive elimination (Saytzew orientation); nor steroids with NH2 groups not adjacent to a bridgehead, like aliphatic amino groups, undergo deamination with predominant inversion of configuration accompanied by some elimination. Cholestanol (11 g.) oxidized 2.5 hrs. at 70-5° with 11.5 g. CrO3 in 90% AcOH gave 8.5 g. 2,3-seco-5α-cholestane-2,3-dioic acid, m. 196-7° (Et2O-pentane), which when refluxed with Ac2O and distilled at 300°/1.5 mm. gave 4.6 g. A-nor-5α-cholestan-2-one (I), m. 100-1° (MeOH); oxime m. 201-3° (EtOAc). I by reduction with excess Na in alc., or with (iso-PrO)3Al in slowly distilling (7 hrs.) PrOH gave a mixture of epimeric alcs., which were separated by overnight treatment with 4% alc. solution of digitonin. The insol. digitonide on decomposition with C5H5N gave A-nor-5α-cholestan-2α-ol (II), m. 128°, [α]D 38° (c 1.2, all rotations determined in CHCl3); acetate, m. 80°, [α]D 1° (c 0.8). The material not precipitated by digitonin gave A-nor-5α-cholestan-2β-ol (III), as solvate, m. 120° with transition to needles m. 135°, and after sublimation at 160°/0.5 mm., m. 153°, [α]D 28° (c 1.0); acetate m. 93°, [α]D 25° (c 0.4). I oxime (0.6 g.) refluxed 2 hrs. in 200 cc. AmOH saturated with Na, left 1.5 hrs., and excess Na destroyed with alc. gave 580 mg. of oil which was chromatographed on Al2O3 to give 430 mg. 2β-amino-A-nor-5α-cholestane (IV), b0.01 150°, [α]D 25.5° (c 0.9); acetyl derivative m. 190-1° (Me2CO), [α]D 39° (c 1.0). I oxime (0.5 g.) hydrogenated 6 hrs. with 200 mg. PtO2 in 50 cc. AcOH, the product acetylated, and chromatographed on Al2O3 gave 410 mg. IV N-Ac derivative 3,4-Seco-5-cholestene-3,4-dioic acid (m. 296°) was converted by refluxing with Ac2O and pyrolyzing at 300-20°/ 1.5 mm. into A-nor-5β-cholesten-3-one (V), m. 95°. Hydrogenation of V with PdO in Et2O-AcOH gave A-nor-5β-cholestan-3-one (VI), m. 74°; oxime m. 129-30°, [α]D 74° (c 0.9). VI (250 mg.) in refluxing alc. treated 2 hrs. with Na, isolated, and chromatographed on Al2O3 gave 200 mg. A-nor-5β-cholestan-3β-ol (VII), m. 89° and 107°, [α]D 51° (c 0.9). VI (85 mg.) refluxed 1 hr. with 50 mg. LiAlH4 in Et2O gave 85 mg. of an oil which when chromatographed gave 69 mg. VII. VI (100 mg.) resisted hydrogenation in the presence of 44 mg. PtO2 in Et2O-AcOH containing 2 drops 60% HClO4 and was

recovered unchanged (97 mg.). V oxime (0.6 g.) refluxed 3 hrs. in 120 cc. AmOH saturated with Na, left 1 hr., excess Na destroyed, and the mixture poured into H2O, extracted with Et2O, and worked up through the Et2O-insol. HCl salt gave 400 mg. 3β-amino-A-nor-5β-cholestane (VIII), b0.5 181-5°, [α]D 46° (c 0.8); Ac derivative m. 246-7°, [α]D 48° (c 0.9). V oxime (250 mg.) reduced 0.75 hr. in 35 cc. AcOH with 100 mg. PtO2 and H gave 220 mg. of an oil which when chromatographed on Al2O3 gave 3α-amino-A-nor-5β-cholestane (IX), m. 66-8° (MeOH), [α]D 9° (c 1.1); Ac derivative m. 166-8°, [α]D 67° (c 0.9). 3β-Hydroxy-6,7-seco-5α-cholestane-6,7-dioic acid, m. 239°, was oxidized with CrO3 in AcOH to the 3-oxo acid, m. 254-5°. The 3-oxo acid (8.3 g.) refluxed 1 hr. with 215 cc. (CH2OH)2 containing 7 cc. N2H4.H2O with 8.3 g. Na, the temperature allowed to rise to 185° and refluxing continued 6 hrs. gave 7.3 g. 6,7-seco-5α-cholestane-6,7-dioic acid (X), m. 272-3° (AcOH). The Ba salt of X by pyrolysis 3 hrs. at 400-20°/1.5 mm. gave B-nor-5β,8α-cholestan-6-one (XI), m. 92-3° (aqueous Me2CO); oxime m. 185-7° (MeOH). XI (200 mg.) refluxed 1.5 hrs. in 80 cc. AmOH with Na and the crude product chromatographed gave 144 mg. B-nor-5β,8α-cholestan-6α-ol (XII), m. 85-7° (aqueous Me2CO), [α]D 42° (c 1.0). XI (300 mg.) refluxed 14 hrs. with excess LiAlH4 and the 290 mg. of crude product chromatographed on Al2O3 gave 145 mg. unchanged XI and 120 mg. XII. XII left overnight with SOCl2 in C5H5N gave B-nor-8α-cholest-5-ene, an oil. XI oxime (215 mg.) refluxed 4 hrs. with Na and AmOH gave after chromatography 6α-amino-B-nor-5β,8α-cholestane (XIII), b1 220-30°, [α]D 33° (c 1.1); Ac derivative, b0.4 180-90°, m. 178-80° (Me2CO), [α]D 14° (c 1.1).
XI oxime (110 mg.) in 30 cc. dioxane refluxed 16 hrs. with excess LiAlH4 and the crude product acetylated and chromatographed gave XIII Ac derivative
XI oxime (120 mg. resisted hydrogenation in 30 cc. AcOH with 50 mg. PtO2 at 20° and at 55-60° with 4 drops 60% HClO4.
5α-Androstan-17-one oxime (XIV) (1 g.) similarly treated with Na in alc. gave 17β-amino-5α-androstane (XV), m. 138-41° (Me2CO); Ac derivative m. 208-9° (EtOAc). XIV (0.5 g.) in 100 cc. Et2O refluxed 3 hrs. with 1 g. LiAlH4 gave 480 mg. XV. XIV (0.4 g.) hydrogenated 1 hr. with 50 cc. AcOH, 100 mg. PtO2, and 2 drops 60% HClO4 gave 380 mg. XV. 3β-Acetoxy-5-androsten-17-one oxime (XVI) (1.5 g.) similarly reduced with 100 cc. alc. and Na gave 1.3 g. 17β-amino-5-androsten-3β-ol (XVII), m. 160° (EtOAc), [α]D -80° (c 1.0); N,O-di-Ac derivative m. 196°, [α]D -88° (c 0.5). XVI (0.5 g.) in 50 cc. Et2O refluxed 3 hrs. with excess LiAlH4 gave 450 mg. XVII. 3β-Acetoxy-5-etienic acid (0.5 g.) in 20 cc. C6H6 refluxed 2 hrs. with 1 cc. purified SOCl2, the chloride in 60 cc. 2:1 Me2CO-dioxane treated 0.5 hr. with 300 mg. NaN3 in 1.2 cc. H2O, and this material heated 1.5 hrs. in C6H6 gave the 17β-isocyanate, which was refluxed 2 hrs. with 20 cc. AcOH and 7 cc. concentrated HCl, evaporated, and the product refluxed 1 hr. with 15% MeOHNaOH, and the base isolated through the Et2O-insol. HCl salt and chromatographed to give 175 mg. XVII. In the following 6 expts. the steroid amine was dissolved in 50% AcOH and where necessary dioxane added to give full solution NaNO2 (2-3 times the weight of amine) in 50% AcOH was added dropwise at 20°, the mixture left overnight, after basification with 4N NaOH, and the product isolated by extraction with Et2O, and then hydrolysis 0.5 hr. with 5% MeOH-KOH, or acetylation at 100°. (1) IV (205 mg.) gave a product which by chromatography on Al2O3 gave 5 mg. of an oil which did not crystallize, but gave a pos. test for unsatn. with C(NO2)4 in CHCl3, and is probably A-nor-5α-cholest-1(and/or -2)-ene, 125 mg. of II, and 60 mg. of an oil which by acetylation gave IV Ac derivative (2) VIII (0.6

g.) gave a product from which most of the basic material was separated by treatment with dry HCl in Et2O. The Et2O-insol. HCl salt (290 mg.) gave on acetylation VIII Ac derivative The 315 mg. of residue by chromatography gave: (a) 177 mg. A-norcholest-3(5)-ene (XVIII), m. 80°, [α]D 53° (c 1.1); (b) 119 mg. VII; and (c) 14 mg. of oil, which on acetylation gave VII Ac derivative (3) IX (210 mg.) gave 195 mg. of crude product which on chromatography gave (a) 82 mg. XVIII, and (b) 105 mg. oils which on acetylation gave IX Ac derivative (4) XIII (300 mg.) gave 280 mg. crude product which on chromatography gave (a) 50 mg. B-nor-8α-cholest-5-ene, noncryst. but gave a pos. C(NO2)4 test; (b) 146 mg. of a substance, C26H46ON2, m. 121° and 136-8°, and (c) 75 mg. of oil which on acetylation gave XIII Ac derivative (5) XV (130 mg.) gave 125 mg. 5α-androstan-17β-ol, m. 168-70° (hexane). (6) XVII (0.5 g.) gave 485 mg. androst-5-ene-3β,17β-diol, m. 177-80° (EtOAc). Complete absence of elimination products in the deamination of 17β-amino steroids may reflect the presence of the angular Me group on the adjacent bridgehead C atom and suggests that a diazonium ion, rather than a carbonium ion, is the important intermediate.

IT Steroids
(Walden inversion and)

IT Walden inversion
(in steroids)

IT Deamination
(of A-nor-, B-nor- and 17-aminosteroids)

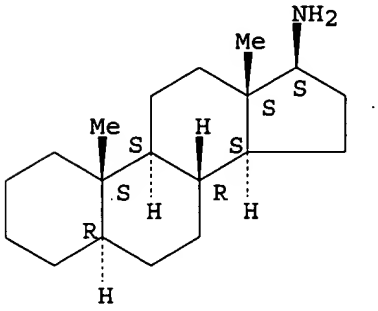
IT 521-17-5, Androst-5-ene-3β,17β-diol 1178-00-3, 1H-Benz[e]indene-6,7-diacetic acid, 3-(1,5-dimethylhexyl)dodecahydro-3a,6-dimethyl- 1178-00-3, 2,3-Seco-5α-cholestane-2,3-dioic acid 2310-36-3, A-Nor-5α-cholestan-2-one 2311-96-8, A-Nor-5α-cholestan-2α-ol 2493-92-7, A-Nor-5α-cholestan-2α-ol, acetate 4350-66-7, Androst-5-en-3β-ol, 17β-amino- 4350-67-8, Androst-5-en-3β-ol, 17β-acetamido-, acetate 6908-01-6, A-Nor-5β-cholestan-3-one 14772-37-3, A-Nor-5α-cholestan-2β-ol 14772-59-9, A-Nor-5α-cholestan-2β-ol, acetate 20853-64-9, 5α-Androstane, 17β-acetamido- 28097-22-5, 4-Indancarboxylic acid, 5-(2-carboxy-1-methyl-4-oxocyclohexyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl- 29599-03-9, 4-Indancarboxylic acid, 5-(2-carboxy-1-methylcyclohexyl)-1-(1,5-dimethylhexyl)hexahydro-7a-methyl- **31239-17-5**, 5α-Androstan-17β-amine 35878-83-2, A-Norcholest-3(5)-ene 56997-89-8, A-Norcholest-5-en-3-one 70182-75-1, A-Nor-5α-cholestan-2-one, oxime 85198-44-3, A-Nor-5β-cholestan-3β-ol 103366-02-5, B-Nor-5β,8α-cholestan-6-one 110346-39-9, 6,7-Seco-5α-cholestane-6,7-dioic acid, 3-oxo- 119677-75-7, B-Nor-8α-cholest-5-ene 122386-63-4, A-Nor-5α-cholestane, 2β-acetamido- 122386-64-5, A-Nor-5β-cholestane, 3α-acetamido- 122386-65-6, A-Nor-5β-cholestane, 3β-acetamido- 122386-75-8, A-Nor-5α-cholest-1-ene 122386-76-9, A-Nor-5α-cholest-2-ene 122386-85-0, B-Nor-5β,8α-cholestane, 6α-acetamido- 122386-90-7, B-Nor-5β,8α-cholestan-6-one, oxime 122441-37-6, A-Nor-5β-cholestan-3-one, oxime 122441-42-3, B-Nor-5β,8α-cholestan-6α-ol 122564-84-5, 6,7-Seco-5α-cholestane-6,7-dioic acid 122626-62-4, B-Nor-5β,8α-cholestan-6α-amine 122650-16-2, A-Nor-5α-cholestan-2β-amine 122650-17-3, A-Nor-5β-cholestan-3α-amine 122650-18-4, A-Nor-5β-cholestan-3β-amine
(preparation of)

IT 217-04-9, Dicyclopenta[a,f]naphthalene 240-05-1, Cyclopenta[a]fluorene
(steroid derivs.)

IT **31239-17-5**, 5α-Androstan-17β-amine
(preparation of)

RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

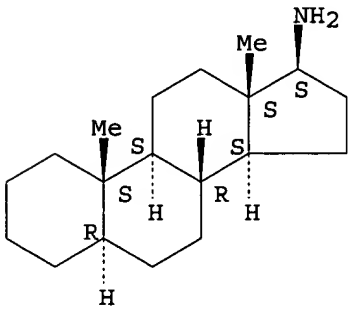


=> d all tot hitstr l34

L34 ANSWER 1 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2004:541472 HCAPLUS
DN 141:350323
ED Entered STN: 07 Jul 2004
TI Conversion of Epiandrosterone Into 17β-Amino-5α-androstane
AU Merlani, M. I.; Davitishvili, M. G.; Nadaraia, N. Sh.; Sikharulidze, M. I.; Papadopulos, K.
CS I. G. Kutateladze Institute of Pharmaceutical Chemistry, Academy of Sciences of Georgia, Tbilisi, 0159, Russia
SO Chemistry of Natural Compounds (Translation of Khimiya Prirodnykh Soedinenii) (2004), 40(2), 144-146
CODEN: CHNCA8; ISSN: 0009-3130
PB Kluwer Academic/Consultants Bureau
DT Journal
LA English
CC 32-4 (Steroids)
AB A new method for synthesizing 17β-amino-5α-androstane was developed based on tigogenin. The configuration at C-17 was proved by PMR.
ST amino androstane prepn
IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(amino; preparation of 17β-amino-5α-androstane from epiandrosterone)
IT Amines, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(steroidal; preparation of 17β-amino-5α-androstane from epiandrosterone)
IT 481-29-8, Epiandrosterone
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of 17β-amino-5α-androstane from epiandrosterone)
IT 963-75-7P 6020-90-2P 10429-07-9P 774604-56-7P 774604-57-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of 17β-amino-5α-androstane from epiandrosterone)
IT **31239-17-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 17β-amino-5α-androstane from epiandrosterone)

RE.CNT 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Babcock, J; US 2863885 1958 HCAPLUS
(2) Babcock, J; US 3009925 1961 HCAPLUS
(3) Campbell, T; Brit J Pharmacol 1982, V76, P337 HCAPLUS
(4) Choppe, C; J Chem Soc 1959, P345
(5) Kemertelidze, E; Khim-Farm Zh 1972, V6(12), P44 HCAPLUS
(6) Kruizinga, W; J Org Chem 1981, V46, P4321 HCAPLUS
(7) Lucas, R; J Am Chem Soc 1960, V82(21), P5688
(8) Marker, R; J Am Chem Soc 1936, V58, P480 HCAPLUS
(9) Nadaraia, N; Zh Org Khim 1987, V23(3), P533 HCAPLUS
(10) Takasuto, S; Chem Pharm Bull 1989, V23(12), P1431
IT **31239-17-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of 17β-amino-5α-androstane from epiandrosterone)
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 2 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2003:912849 HCAPLUS
DN 139:374985
ED Entered STN: 21 Nov 2003
TI Therapeutic compositions using androstane amides effective against Gram-positive bacteria
IN **Pettit, George R.; Pettit, Robin K.**
PA USA
SO U.S. Pat. Appl. Publ., 12 pp.
CODEN: USXXCO
DT Patent
LA English
IC ICM A61K031-56
ICS A61K031-58
INCL 514176000; 514182000
CC 1-5 (Pharmacology)
Section cross-reference(s): 63
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2003216361	A1	20031120	US 2001-893861	20010628 <--
PRAI US 2000-214844P	P	20000628 <--		

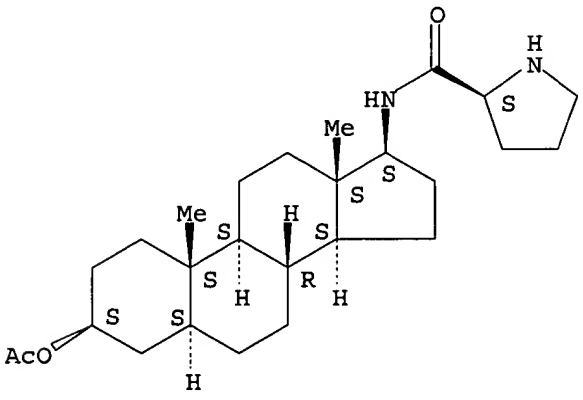
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
US 2003216361	ICM	A61K031-56

ICS A61K031-58
INCL 514176000; 514182000
US 2003216361 NCL 514/176.000
ECLA A61K031/56; A61K031/58 <--
OS MARPAT 139:374985
AB The invention discloses androstane amide compds., especially **3. beta.-acetoxy-17β -(L-prolyl)amino-5α - androstane.** The compds. are useful as antimicrobial agents, most specifically against Gram- pos. bacteria. The invention further discloses pharmaceutical compns. and methods of treating bacterial infection using such compns.
ST androstane amide deriv antibacterial Gram pos bacteria; prolyl androstane deriv antibacterial Gram pos bacteria
IT Antibacterial agents
Antibiotic resistance
Arcanobacterium haemolyticum
Bacillus cereus
Bacillus circulans
Bacillus licheniformis
Bacillus subtilis
Bactericide resistance
Candida albicans
Corynebacterium diphtheriae
Corynebacterium hoagii
Cryptococcus neoformans
Drug delivery systems
Enterobacter cloacae
Enterococcus
Enterococcus faecalis
Enterococcus faecium
Escherichia coli
Firmicutes
Gardnerella vaginalis
Gordonia bronchialis
Gordonia sputi
Klebsiella pneumoniae
Lactobacillus
Listeria monocytogenes
Micrococcus luteus
Neisseria gonorrhoeae
Nocardia asteroides
Nocardia farcinica
Paenibacillus alvei
Proteus vulgaris
Pseudomonas aeruginosa
Rhodococcus
Rhodococcus equi
Staphylococcus aureus
Staphylococcus epidermidis
Staphylococcus saprophyticus
Stenotrophomonas maltophilia
Streptococcus group A
Streptococcus pneumoniae
(androstane amides effective against Gram-pos. bacteria)
IT Antimicrobial agents
(androstane amides effective against Gram-pos. bacteria, and use with other antimicrobial agents)
IT Infection
(bacterial; androstane amides effective against Gram-pos. bacteria)

IT Medical goods
(dressings, surface-adhering; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(emulsions; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(lotions; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(oily; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(ointments, creams; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(ointments; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(salves; androstane amides effective against Gram-pos. bacteria)
IT Mutation
(spontaneous mutants; androstane amides effective against Gram-pos. bacteria)
IT Drug delivery systems
(topical; androstane amides effective against Gram-pos. bacteria)
IT 438-22-2D, Androstane, derivs. **13574-69-1**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(androstane amides effective against Gram-pos. bacteria)
IT 61-32-5, Methicillin 1404-90-6, Vancomycin 1406-05-9, Penicillin
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(resistance to; androstane amides effective against Gram-pos. bacteria)
IT **13574-69-1**
RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(androstane amides effective against Gram-pos. bacteria)
RN 13574-69-1 HCAPLUS
CN 2-Pyrrolidinecarboxamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 3 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:526375 HCAPLUS
DN 133:203156
ED Entered STN: 02 Aug 2000
TI Antimicrobial and cancer cell growth inhibitory activities of 3.

beta.-acetoxy-17β -(L-prolyl)amino-5α -androstane in vitro

AU **Pettit, R. K.**; Cage, G. D.; **Pettit, G. R.**; Liebman, J. A.
CS Cancer Research Institute, Departments of Microbiology and Chemistry, Arizona State University, Tempe, AZ, 85287-1604, USA

SO International Journal of Antimicrobial Agents (**2000**), 15(4), 299-304
CODEN: IAAGEA; ISSN: 0924-8579
PB Elsevier Science Ireland Ltd.
DT Journal
LA English
CC 2-4 (Mammalian Hormones)

AB The in vitro activity of the steroidal amide **3β -acetoxy-17β -(L-prolyl)amino-5α -androstane** against 179 Gram-pos. clin. isolates was examined The min. bactericidal concentration (MBC)/MIC ratios were ≤2 for 73% of methicillin-resistant Staphylococcus aureus, 59% of vancomycin-resistant Enterococcus spp. and 88% of penicillin-resistant Streptococcus pneumoniae. The androstane derivative was bactericidal for a variety of other Gram-pos. genera, including Nocardia, Corynebacterium and Listeria. Variation in MICs is pH 6-8 media was slight. The frequency of occurrence of bacterial spontaneous mutations to resistance ranged from 10-6 to 10-9. Kill curve anal. confirmed the bactericidal nature of the steroidal amide, and demonstrated that killing was time dependent but not concentration dependent for all organisms. The ability of **3β -acetoxy-17β -(L-prolyl)amino-5α -androstane** to inhibit human cancer cell growth was also evaluated. The concentration required to inhibit 50% of cell growth (GI50) was <2.5 mg/l for all cell lines examined In single-dose murine toxicity evaluations, the androstane derivative was non-toxic at doses up to 400 mg/kg.

ST androstane amide antimicrobial antitumor cancer cell proliferation inhibition toxicity

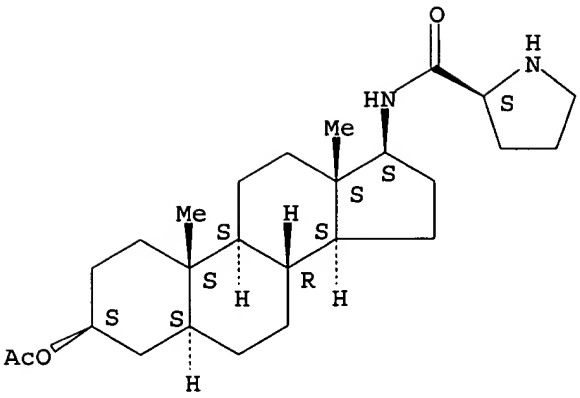
IT Antimicrobial agents
Antitumor agents
Corynebacterium
Enterococcus faecalis
Listeria
Nocardia
Ovary, neoplasm
Pancreas, neoplasm
Proliferation inhibition
Rhodococcus
Staphylococcus aureus
Streptococcus pneumoniae
(**3β -acetoxy-17β -(L-prolyl)amino-5α -androstane** in vitro antimicrobial and cancer cell growth inhibition activity and in vivo murine toxicity)

IT Nervous system
(central, neoplasm; **3β -acetoxy-17β -(L-prolyl)amino-5α -androstane** in vitro antimicrobial and cancer cell growth inhibition activity and in vivo murine toxicity)

IT Intestine, neoplasm
(colon; **3β -acetoxy-17β -(L-prolyl)amino-5**

α -**androstane** in vitro antimicrobial and cancer
cell growth inhibition activity and in vivo murine toxicity)
IT Leukemia
(lymphocytic; 3β -**acetoxy-17**
β -(L-**prolyl**)**amino-5**
α -**androstane** in vitro antimicrobial and cancer
cell growth inhibition activity and in vivo murine toxicity)
IT Prostate gland
(neoplasm; 3β -**acetoxy-17**
β -(L-**prolyl**)**amino-5**
α -**androstane** in vitro antimicrobial and cancer
cell growth inhibition activity and in vivo murine toxicity)
IT Lung, neoplasm
(non-small-cell carcinoma; 3β -**acetoxy**
-17β -(L-**prolyl**)**amino-**
5α -**androstane** in vitro antimicrobial
and cancer cell growth inhibition activity and in vivo murine toxicity)
IT **13574-69-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3β -**acetoxy-17**
β -(L-**prolyl**)**amino-5**
α -**androstane** in vitro antimicrobial and cancer
cell growth inhibition activity and in vivo murine toxicity)
RE.CNT 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Amyes, S; J Med Microbiol 1997, V46, P436 HCAPLUS
(2) Anon; Dictionary of Antibiotics and Related Substances 1988
(3) Koll, B; Clin Infect Dis 1993, V17(Suppl 2), PS322
(4) Monks, A; J Natl Cancer Inst 1991, V83, P757 HCAPLUS
(5) National Committee for Clinical Laboratory Standards; Approved Standard M2-A6 1997
(6) National Committee for Clinical Laboratory Standards; Approved standard M7-A4 1997
(7) Pettit, G; J Med Chem 1967, V10, P145 HCAPLUS
(8) Pfaller, M; Antimicrob Agents Chemother 1998, V42, P1762 HCAPLUS
IT **13574-69-1**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(3β -**acetoxy-17**
β -(L-**prolyl**)**amino-5**
α -**androstane** in vitro antimicrobial and cancer
cell growth inhibition activity and in vivo murine toxicity)
RN 13574-69-1 HCAPLUS
CN 2-Pyrrolidinecarboxamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 4 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1992:490139 HCAPLUS
DN 117:90139
ED Entered STN: 05 Sep 1992
TI Preparation of indole-3-methanamines useful as antidiabetic, antiobesity and antiatherosclerotic agents
IN Lin, Chiu Hong; Sih, John Charles; Tanis, Steven Paul
PA Upjohn Co., USA
SO PCT Int. Appl., 77 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07D209-14
ICS A61K031-40; C07D405-12; C07D491-04
CC 27-11 (Heterocyclic Compounds (One Hetero Atom))
Section cross-reference(s): 1
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9207829	A1	19920514	WO 1991-US7785	19911029 <--
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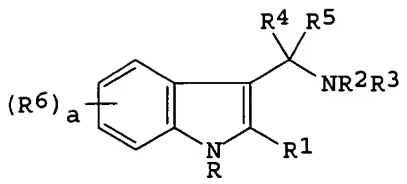
	RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FR, GA, GB, GN, GR, IT, LU, ML, MR, NL, SE, SN, TD, TG				
	AU 9188765	A1	19920526	AU 1991-88765	19911029 <--
PRAI	US 1990-608159	A2	19901102 <--		
	WO 1991-US7785	A	19911029 <--		

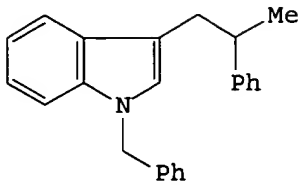
CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES
WO 9207829	ICM	C07D209-14
	ICS	A61K031-40; C07D405-12; C07D491-04

OS MARPAT 117:90139
GI



I



II

AB Title compds. [I; R = alkyl, alkenyl, alkynyl, R1CO, (substituted) Ph, PhCH2, PhSO2, carbamoyl, aminoalkyl, etc.; R1 = H, alkyl, alkenyl, alkynyl, (substituted) Ph, PhCH2; R2 = (substituted) PhCH2, furylmethyl, thienylmethyl, pyridylmethyl, pyrrolylmethyl, indolylmethyl, benzofurylmethyl, imidazolylmethyl, etc.; R3 = H, (substituted) PhCH2; R4 = H, CH2OH; R5 = H, alkyl, hydroxyalkyl; R6 = H, halo, OH, OR8, SR8, NO2, amino, O2CR1, COR1, CF3, R7R8NSO2, SR8, cyano, R5O2C, alkyl, etc.; R7 = H, alkyl; R8 = H, alkyl, alkenyl, alkynyl, (substituted) Ph, PhCH2, cycloalkyl, cycloalkylmethyl, etc.], also useful as antihyperglycemics (no data) were prepared Thus, (S)-α-methylbenzylamine, 1-benzyl-1H-indole-3-carboxaldehyde (preparation given), and NaBH3CN were stirred 48 h in MeOH/HOAC to give (S)-II.

ST indolemethanamine prepn antidiabetic; antiobesity agent indolemethanamine; antihyperlipidemic indolemethanamine

IT Antidiabetics and Hypoglycemics
Antiobesity agents
(indolemethanamines)

IT Arteriosclerosis
(atherosclerosis, treatment of, indolemethanamines for)

IT **31239-17-5**, 17-Aminoandrostane
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of indolecarboxaldehyde derivative)

IT 64-04-0, 2-Phenylethylamine 64715-80-6 64715-85-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with indolecarboxaldehyde derivative)

IT 2740-83-2, 3-Trifluoromethylbenzylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with indolecarboxaldehyde derivative, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 35019-66-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with methylindolecarboxaldehyde)

IT 50-99-7, D-Glucose, biological studies
RL: BIOL (Biological study)
(impaired tolerance to, treatment of, indolemethanamines for)

IT 9004-10-8, Insulin, biological studies
RL: BIOL (Biological study)
(insensitivity to, treatment of, indolemethanamines for)

IT 95-87-4, 2,5-Dimethylphenol
RL: RCT (Reactant); RACT (Reactant or reagent)
(nitration of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 142769-46-8P 142769-47-9P 142769-48-0P 142769-49-1P 142769-50-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyanoborohydride reduction of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 62492-45-9P 63762-72-1P 142769-25-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 59382-36-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive amination of indolecarboxaldehyde derivative by, as intermediate for antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 10511-51-0P, 1-Benzylindole-3-carboxaldehyde
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive amination of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 142769-44-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reductive amination of, in preparation of intermediate for antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 56026-56-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and salification of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 142768-86-3P 142768-87-4P 142768-88-5P 142768-89-6P 142768-90-9P
142768-91-0P 142768-92-1P 142768-93-2P 142768-94-3P 142768-95-4P
142768-96-5P 142768-97-6P 142768-98-7P 142768-99-8P 142769-00-4P
142769-01-5P 142769-02-6P 142769-03-7P 142769-04-8P 142769-05-9P
142769-06-0P 142769-07-1P 142769-08-2P 142769-09-3P 142769-10-6P
142769-11-7P 142769-12-8P 142769-13-9P 142769-14-0P 142769-15-1P
142769-16-2P 142769-17-3P 142769-18-4P 142769-19-5P 142769-20-8P
142769-21-9P 142769-22-0P 142769-23-1P 142769-24-2P 142769-45-7P
142797-36-2P 142807-47-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 142769-39-9P 142769-42-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as antidiabetic, antiobesity, and antiatherosclerotic agent agent)

IT 61019-04-3P 63762-71-0P 63762-82-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 267-48-1P, 5H-1,3-Dioxolo[4,5-f]indole 3139-05-7P 3139-06-8P
3139-10-4P 4581-84-4P 6953-22-6P 10601-19-1P 13429-10-2P
16382-21-1P 16382-24-4P 32996-27-3P 39974-94-2P 40130-97-0P
61019-03-2P 61019-05-4P 63762-79-8P 63762-80-1P 63762-81-2P
63762-83-4P 68935-52-4P 77248-65-8P 101966-88-5P 104831-78-9P
104831-79-0P 142768-85-2P 142769-26-4P 142769-27-5P 142769-28-6P
142769-29-7P 142769-30-0P 142769-31-1P 142769-33-3P 142769-34-4P
142769-35-5P 142769-36-6P 142769-37-7P 142769-38-8P 142769-40-2P
142769-41-3P 142769-43-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for antidiabetic, antiobesity, and antiatherosclerotic agents)

IT 95-87-4, 2,5-Dimethylphenol 100-44-7, Benzyl chloride, reactions

124-40-3, Dimethylamine, reactions 349-76-8 487-89-8,
1H-Indole-3-carboxaldehyde 615-74-7, 2-Chloro-5-methylphenol
1006-94-6, 5-Methoxyindole 1215-59-4 2835-98-5, 6-Amino-m-cresol
4637-24-5, DMF dimethyl acetal 7145-99-5, 3,4-Methylenedioxytoluene
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 10075-50-0, 5-Bromoindole
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with methiothiocopper, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 3300-51-4, p-Trifluoromethylbenzylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive amination by, of indolecarboxaldehyde deriv)

IT 100-46-9, Benzylamine, reactions 100-81-2, 3-Methylbenzylamine
109-12-6, 2-Aminopyrimidine 617-89-0, Furfurylamine 618-36-0,
α-Methylbenzylamine 2393-23-9, 4-Methoxybenzylamine 18469-52-8
20989-17-7, (S)-Phenylglycinol 56613-80-0, R-Phenylglycinol
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive amination by, of indolecarboxaldehyde derivative)

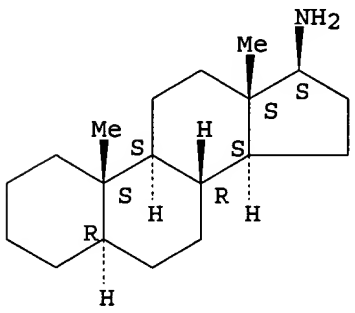
IT 19012-03-4, 1-Methylindole-3-carboxaldehyde 142769-51-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive amination of, in preparation of antidiabetic, antiobesity, and antiatherosclerotic agent)

IT 3886-69-9, R-α-Methylbenzylamine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reductive condensation of, with indolecarboxaldehyde derivative)

IT **31239-17-5**, 17-Aminoandrostane
RL: RCT (Reactant); RACT (Reactant or reagent)
(amination by, of indolecarboxaldehyde derivative)

RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 5 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1988:75714 HCAPLUS
DN 108:75714
ED Entered STN: 05 Mar 1988
TI Steroids and their cyclic hydrocarbon analogs with amino-containing sidechains, useful as antidiabetic agents and inhibitors of phospholipase A2
IN Johnson, Roy A.; Bundy, Gordon L.; Youngdale, Gilbert A.; Morton, Douglas R.
PA Upjohn Co. , USA
SO PCT Int. Appl., 177 pp.

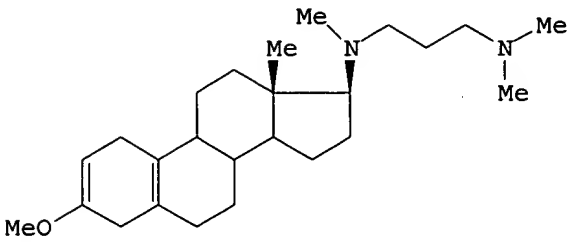
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J041-00
ICS C07J043-00; A61K031-56; A61K031-58; C07C087-34; C07C087-455; C07D213-38; C07F009-24; C07F009-22; A61K031-13
CC 32-3 (Steroids)
Section cross-reference(s): 1, 2
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 8702367	A2	19870423	WO 1986-US2116	19861007	<--
	WO 8702367	A3	19880630			
	W: JP, US, US					
	RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE					
	EP 243449	A1	19871104	EP 1986-906569	19861007	<--
	R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE					
	JP 63501217	T2	19880512	JP 1986-505710	19861007	<--
	US 4917826	A	19900417	US 1987-117851	19870616	<--
	US 5196542	A	19930323	US 1991-657721	19910220	<--
	US 5145874	A	19920908	US 1991-663037	19910225	<--
	US 5187299	A	19930216	US 1991-793486	19911113	<--
	US 5274089	A	19931228	US 1992-972693	19921106	<--
	US 5334712	A	19940802	US 1992-976751	19921116	<--
	US 5373095	A	19941213	US 1993-126153	19930923	<--
	US 5621123	A	19970415	US 1994-247169	19940520	<--
PRAI	US 1985-788995	A2	19851018	<--		
	US 1986-843120	A2	19860324	<--		
	WO 1986-US2116	W	19861007	<--		
	US 1987-117851	A3	19870616	<--		
	US 1989-394396	A3	19890815	<--		
	US 1991-657721	A3	19910220	<--		
	US 1991-657729	B1	19910220	<--		
	US 1991-793486	A3	19911113	<--		
	US 1992-972693	A3	19921106	<--		
	US 1992-976751	A3	19921116	<--		

CLASS

PATENT NO.	CLASS	PATENT FAMILY CLASSIFICATION CODES	
WO 8702367	ICM	C07J041-00	
	ICS	C07J043-00; A61K031-56; A61K031-58; C07C087-34; C07C087-455; C07D213-38; C07F009-24; C07F009-22; A61K031-13	
US 4917826	NCL	552/522.000; 514/169.000; 514/182.000; 514/237.800; 514/253.020; 514/351.000; 514/352.000; 514/381.000; 514/398.000; 514/399.000; 514/400.000; 514/424.000; 514/426.000; 514/471.000; 514/472.000; 514/866.000; 544/154.000; 544/380.000; 546/300.000; 546/304.000; 546/307.000; 546/312.000	<--
US 5196542	NCL	546/326.000; 540/107.000; 546/333.000; 564/460.000	<--
US 5145874	NCL	514/650.000; 514/529.000; 514/532.000; 514/533.000; 514/534.000; 514/538.000; 514/545.000; 514/579.000; 514/613.000; 514/616.000; 514/617.000; 514/618.000; 514/619.000; 514/620.000; 514/621.000; 514/622.000; 514/623.000; 514/642.000; 564/281.000; 564/337.000; 564/453.000; 564/454.000; 564/455.000; 564/456.000; 564/461.000	<--
US 5187299	NCL	552/522.000; 552/554.000	<--
US 5274089	NCL	540/112.000; 552/522.000	<--
US 5334712	NCL	540/112.000; 540/117.000; 552/522.000	

ECLA C07C087/28; C07C087/40; C07C103/44; C07C103/737; C07D213/38; C07F009/22C; C07F009/24C1+U; C07J041/00B; C07J041/00C6; C07J041/00C40; C07J043/00B; C07J051/00<--
US 5373095 NCL 540/095.000; 540/106.000
ECLA C07C087/28; C07C087/40; C07C103/44; C07C103/737; C07D213/38; C07F009/22C; C07F009/24C1+U; C07J041/00B; C07J041/00C6; C07J041/00C40; C07J043/00B; C07J051/00<--
US 5621123 NCL 552/522.000; 552/554.000
ECLA C07J041/00B; C07J041/00C6 <--
OS CASREACT 108:75714
GI



I

AB A wide variety of steroids and nonsteroidal analogs bearing amino-containing sidechains were prepared for use as antidiabetic agents and in the treatment or prevention of phospholipase A2-mediated conditions. Reductive amination of estrone Me ether with Me2N(CH2)3NH2 and HCO2H at 160-170° gave N-[3-(dimethylamino)propyl]-N-formyl-3-methoxyestra-1,3,5(10)-trien-17β-amine, which was reduced by LiAlH4 in dioxane to the N-Me derivative This underwent Birch reduction, followed by 3 recrystns. in Et2O-MeCN, to give estradienamine derivative I. In the perfused guinea pig lung, I completely inhibited phospholipase A2 at 4 + 10-7 M.

ST amino steroid prepn antidiabetic phospholipase inhibitor; estranamine prepn antidiabetic phospholipase inhibitor

IT Antidiabetics and Hypoglycemics
(amino steroids and analogs)

IT Steroids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(amino, preparation of, and analogs, as phospholipase A2 inhibitors and antidiabetic agents)

IT 9001-84-7, Phospholipase A2
RL: RCT (Reactant); RACT (Reactant or reagent)
(inhibitors of, amino-containing steroids and analogs as)

IT 53-44-1P 1434-85-1P, 17β-Hydroxy-5α-estran-3-one 1624-73-3P 5997-25-1P 30933-83-6P 40216-82-8P, Ornithine methyl ester dihydrochloride 57133-29-6P 75950-19-5P 76555-98-1P 112646-79-4P 112647-70-8P 112648-94-9P 112648-95-0P 112648-96-1P 112648-97-2P 112648-98-3P 112648-99-4P 112649-00-0P 112649-01-1P 112649-02-2P 112649-03-3P 112663-20-4P 112663-21-5P 112663-22-6P 112663-31-7P 112663-33-9P 112663-34-0P 112663-38-4P 112663-39-5P 112663-40-8P 112663-41-9P 112663-42-0P 112663-44-2P 112663-45-3P 112663-46-4P 112663-50-0P 112663-51-1P 112663-52-2P 112663-53-3P 112663-54-4P 112663-55-5P 112663-56-6P 112663-57-7P 112663-58-8P 112663-59-9P 112663-60-2P 112663-61-3P 112663-62-4P 112663-63-5P 112663-67-9P 112693-14-8P 112693-15-9P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)

IT 56-18-8P, 3,3'-Iminobis(propylamine) 26358-84-9P 28336-31-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 2640-80-4P 4536-52-1P 4991-61-1P 4991-63-3P 5668-07-5P
5997-25-1P 6291-85-6P, 3-Ethoxypropylamine 17630-26-1P 17630-27-2P
20432-64-8P 32436-37-6P 57764-88-2P 57764-89-3P 59766-90-4P
96148-91-3P 112646-53-4P 112646-54-5P 112646-55-6P 112646-56-7P
112646-57-8P 112646-58-9P 112646-59-0P 112646-60-3P 112646-62-5P
112646-63-6P 112646-65-8P 112646-67-0P 112646-68-1P 112646-69-2P
112646-70-5P 112646-71-6P 112646-72-7P 112646-73-8P 112646-74-9P
112646-75-0P 112646-76-1P 112646-77-2P 112646-78-3P 112646-79-4P
112646-80-7P 112646-81-8P 112646-82-9P 112646-83-0P 112646-84-1P
112646-85-2P 112646-86-3P 112646-87-4P 112646-88-5P 112646-89-6P
112646-90-9P 112646-91-0P 112646-92-1P 112646-93-2P 112646-94-3P
112646-95-4P 112646-96-5P 112646-97-6P 112646-98-7P 112646-99-8P
112647-00-4P 112647-01-5P 112647-02-6P 112647-03-7P 112647-04-8P
112647-05-9P 112647-06-0P 112647-07-1P 112647-08-2P 112647-09-3P
112647-10-6P 112647-11-7P 112647-12-8P 112647-13-9P 112647-14-0P
112647-15-1P 112647-16-2P 112647-17-3P 112647-18-4P 112647-19-5P
112647-20-8P 112647-21-9P 112647-22-0P 112647-23-1P 112647-24-2P
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112647-68-4P 112647-69-5P 112647-70-8P 112647-71-9P 112647-72-0P
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112648-69-8P 112648-70-1P 112648-71-2P 112648-72-3P 112648-73-4P
112648-74-5P 112648-75-6P 112648-76-7P 112648-77-8P 112648-78-9P
112648-79-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as phospholipase A2 inhibitor and/or antidiabetic agent)

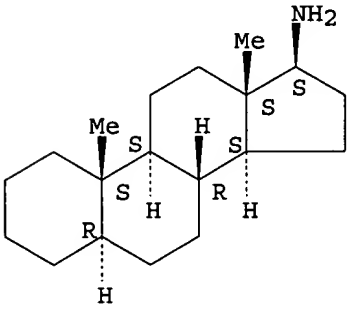
IT 112648-80-3P 112648-81-4P 112648-82-5P 112648-83-6P 112648-84-7P
112648-85-8P 112648-86-9P 112648-87-0P 112648-88-1P 112648-89-2P
112648-90-5P 112648-91-6P 112648-92-7P 112648-93-8P 112649-04-4P

112649-05-5P 112649-06-6P 112663-15-7P 112663-16-8P 112663-17-9P
112663-18-0P 112663-19-1P 112663-23-7P 112663-24-8P 112663-25-9P
112663-26-0P 112663-27-1P 112663-28-2P 112663-29-3P 112663-30-6P
112663-32-8P 112663-35-1P 112663-36-2P 112663-47-5P 112663-48-6P
112663-49-7P 112663-64-6P 112663-65-7P 112663-66-8P 112710-67-5P
112710-68-6P 112710-69-7P 112711-11-2P 112711-12-3P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(preparation of, as phospholipase A2 inhibitor and/or antidiabetic agent)

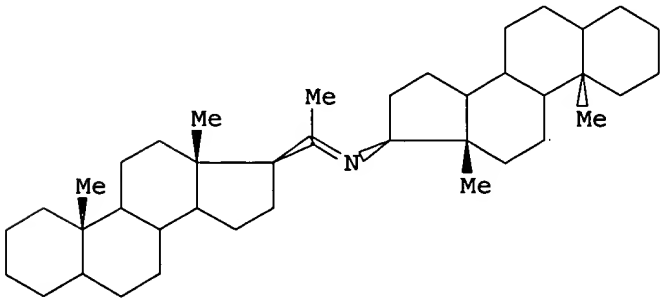
IT 50-28-2, reactions 51-67-2, Tyramine 53-16-7, Estrone, reactions 53-41-8 53-43-0, 3β-Hydroxy-5-androsten-17-one 53-45-2, Estra-1,3,5(10)-trien-17-one 64-04-0, Phenethylamine 64-18-6, reactions 71-44-3, Spermine 75-07-0, reactions 79-04-9 81-25-4 89-97-4, 2-Chlorobenzylamine 90-42-6, 2-Cyclohexyl cyclohexanone 91-00-9, Aminodiphenylmethane 92-68-2, 4-Cyclohexylcyclohexanone 95-00-1, 2,4-Dichlorobenzylamine 96-32-2, Methyl bromoacetate 100-46-9, reactions 100-52-7, reactions 102-49-8, 3,4-Dichlorobenzylamine 104-53-0, Hydrocinnamaldehyde 104-86-9, 4-Chlorobenzylamine 104-88-1, 4-Chlorobenzaldehyde, reactions 105-39-5, Ethyl chloroacetate 107-13-1, reactions 107-85-7, Isoamylamine 108-00-9, unsym-Dimethyl-ethylenediamine 108-31-6, reactions 108-94-1, reactions 109-01-3, N-Methylpiperazine 109-55-7, 3-Dimethylaminopropylamine 109-64-8, 1,3-Dibromopropane 109-76-2, 1,3-Propanediamine 110-13-4, 2,5-Hexanedione 110-60-1, 1,4-Diaminobutane 111-40-0 123-00-2, 3-Morpholinopropylamine 123-38-6, reactions 124-09-4, reactions 124-13-0, Octylaldehyde 124-20-9, Spermidine 124-25-4, Tetradecyl aldehyde 138-14-7 140-75-0, 4-Fluorobenzylamine 140-80-7, 2-Amino-5-diethylaminopentane 156-87-6 327-92-4, 1,5-Difluoro-2,4-dinitrobenzene 333-93-7, 1,4-Diaminobutane dihydrochloride 373-44-4, 1,8-Octanediamine 462-94-2, 1,5-Diaminopentane 502-72-7, Cyclopentadecanone 506-59-2, Dimethylamine hydrochloride 566-88-1, 5α-Cholestan-3-one 590-86-3, Isovaleraldehyde 593-51-1, Methylamine hydrochloride 598-21-0, Bromoacetyl bromide 617-89-0, 2-Aminomethyl-furan 646-25-3, 1,10-Decanediamine 700-58-3, 2-Adamantanone 766-39-2, 2,3-Dimethylmaleic anhydride 814-68-6, Acryloyl chloride 830-13-7, Cyclododecanone 929-06-6, 2-(2-Aminoethoxy)ethanol 963-74-6, 5α-Androstan-17-one 1035-77-4, Estradiol 3-methyl ether 1624-62-0, Estrone methyl ether 1755-52-8 2038-03-1, 2-Morpholinoethylamine 2393-23-9, 4-Methoxybenzylamine 2524-64-3, Diphenyl chlorophosphate 2706-56-1, 2-(2-Aminoethyl)pyridine 2740-83-2, 3-(Trifluoromethyl)benzylamine 3029-19-4, 1-Pyrenecarboxaldehyde 3048-01-9 3179-63-3 3300-51-4, 4-(Trifluoromethyl)benzylamine 3731-51-9, 2-(Aminomethyl)pyridine 3731-52-0, 3-(Aminomethyl)pyridine 3731-53-1, 4-(Aminomethyl)pyridine 4048-33-3, 6-Amino-1-hexanol 4097-89-6, Tris-(2-aminoethyl)amine 4894-75-1 5036-48-6 5104-49-4, Flurbiprofen 5538-95-4, N-Dodecyl-1,3-propanediamine 5625-80-9 5680-79-5, Glycine methyl ester hydrochloride 5993-91-9 6211-16-1 6384-10-7, Ornithine methyl ester 6711-48-4 7149-10-2 7152-51-4 7209-38-3, 1,4-Bis(3-aminopropyl)piperazine 7663-77-6, 1-(3-Aminopropyl)-2-pyrrolidinone 10025-87-3 10517-44-9 13258-63-4, 4-(2-Aminoethyl)pyridine 14210-25-4 19475-35-5 21370-71-8, trans-1-Decalone 27757-85-3, 2-Thiophenemethylamine 28143-91-1 29602-39-9 30525-89-4, Paraformaldehyde **31239-17-5**, 5α-Androstan-17β-amine 34015-48-0, Lysine methyl ester dihydrochloride 35303-76-5, 4-(2-Aminoethyl)benzenesulfonamide 40226-15-1 42014-51-7 49783-80-4 55757-60-3 56183-69-8, Diethyl phosphorohydrazidate 69225-59-8 75659-75-5 83732-75-6, 2-(2-Aminoethyl)-1-methylpyrrole 85666-15-5

112663-37-3 112663-43-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
IT **31239-17-5**, 5α-Androstan-17β-amine
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 6 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1980:181459 HCAPLUS
DN 92:181459
ED Entered STN: 12 May 1984
TI Acid-catalyed decomposition of (20R) and (20S)-20-azido-5α-pregnane: bis steroid Schiff base formation via imine coupling
AU Kabore, I. Z.; Khuong-Huu, Q.; Pancrazi, A.
CS Inst. Chim. Subst. Nat., Gif-sur-Yvette, 91190, Fr.
SO Tetrahedron Letters (**1979**), (28), 2613-14
CODEN: TELEAY; ISSN: 0040-4039
DT Journal
LA English
CC 32-5 (Steroids)
GI

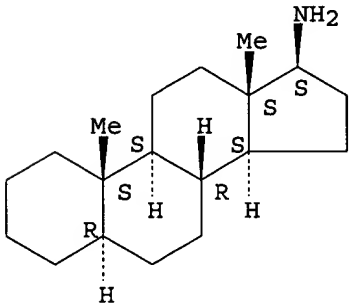


I

AB BF3.Et2O-catalyzed decomposition of the title pregnanes gave, after hydrolysis with aqueous NaOH, 74% Schiff base I. The formation of I involves coupling of an imine intermediate with an iminium complex.

ST coupling azidopregnane decompn; androstanyliminopregnane; pregnane azido decompn coupling
IT Coupling reaction
(of azidoprepnanes during boron trifluoride etherate-catalyzed decomposition)
IT Steroids, reactions
(20-azido, decomposition and steroid coupling reaction of)
IT 14964-30-8 14964-31-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(decomposition and steroid coupling reaction of)
IT 848-62-4P 20853-63-8P **31239-17-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **31239-17-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 7 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1974:552498 HCAPLUS
DN 81:152498
ED Entered STN: 12 May 1984
TI Bromo, chloro, and amino derivatives of 5α-androstane and 5α-estrane
AU Cowell, David B.; Davis, Alan K.; Mathieson, David W.; Nicklin, Paul D.
CS Sch. Pharm., Univ. Bradford, Bradford, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (**1974**), (13), 1505-13
CODEN: JCPRB4; ISSN: 0300-922X
DT Journal
LA English
CC 32-4 (Steroids)
AB 5α-Androstanols and (hydroxyimino)-5α-androstanes gave by standard procedures the chloro-, bromo-, amino-, and acetamido-5α-androstanes. 5α-Estran-17β-ol with PCl5 gave 17α-chloro-5α-estrane.
ST androstane bromo chloro amino; estrane chloro; bromination steroid hydroxy; chlorination steroid hydroxy
IT Steroids, preparation
RL: PREP (Preparation)
(bromo, chloro, and amino)
IT Bromination
Chlorination

(of androstanes)
IT Oximes
RL: SPN (Synthetic preparation); PREP (Preparation)
(steroidal, preparation and reduction of)
IT 7459-06-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(dehydrobromination of)
IT 1032-15-1 1224-92-6 1225-43-0 1476-64-8 17320-50-2 19037-33-3
20311-10-8 20707-77-1 20707-78-2 20707-85-1 25814-80-6
32215-75-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(halogenation of)
IT 35494-01-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of)
IT 2232-18-0 32222-21-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrogenation of, in presence of methanol)
IT 1058-63-5 1254-34-8 54155-80-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of)
IT 7459-05-4P 54156-09-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and halogenation of)
IT 1035-62-7P 14475-43-5P 54156-21-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
IT 1032-14-0P 2872-91-5P 4642-61-9P 7657-50-3P 13067-44-2P
19037-31-1P 20985-60-8P 21002-27-7P 29096-82-0P **31239-17-5P**
31239-23-3P 31239-24-4P 51092-05-8P 54155-78-1P
54155-79-2P 54155-81-6P 54155-82-7P 54155-83-8P 54155-84-9P
54155-85-0P 54155-86-1P 54155-87-2P 54155-88-3P 54155-89-4P
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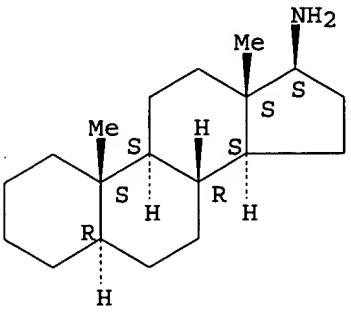
54156-32-0P 54156-33-1P 54156-34-2P 54156-35-3P **54156-36-4P**
54156-37-5P 54156-38-6P 54156-39-7P 54156-40-0P
54156-41-1P 54156-42-2P 54156-43-3P 54156-44-4P 54156-45-5P
54156-46-6P 54156-47-7P 54156-48-8P 54156-49-9P 54165-72-9P
54196-24-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 963-74-6 1032-16-2 1224-95-9 1225-48-5 1755-32-4 3676-06-0
13583-70-5
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with hydrazine)
IT 14546-37-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(reduction of)
IT **31239-17-5P 31239-23-3P 54156-36-4P**
54156-37-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

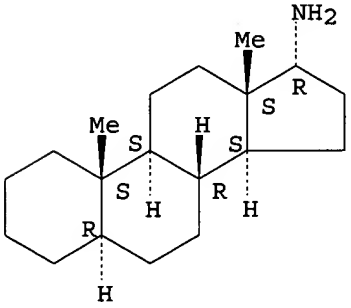
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 31239-23-3 HCAPLUS
CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

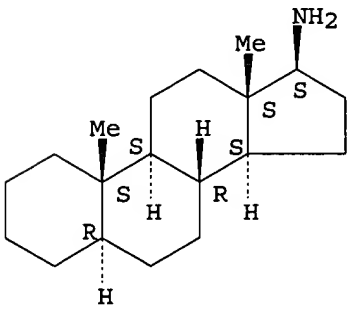


RN 54156-36-4 HCAPLUS
CN Androstan-17-amine, (5α,17β)-, acetate (9CI) (CA INDEX NAME)

CM 1

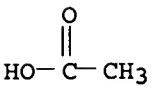
CRN 31239-17-5
CMF C19 H33 N

Absolute stereochemistry.



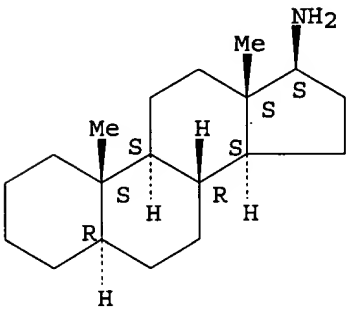
CM 2

CRN 64-19-7
CMF C2 H4 O2



RN 54156-37-5 HCAPLUS
CN Androstan-17-amine, hydrochloride, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

L34 ANSWER 8 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:528415 HCAPLUS
DN 75:128415
ED Entered STN: 12 May 1984
TI Steroids and steroidases. 10. Potentially antitumor active androstane compounds containing C-17 nitrogen mustard functions
AU Jones, J. Bryan; Adam, David J.; Leman, Jeffrey D.
CS Dep. Chem., Univ. Toronto, Toronto, ON, Can.
SO Journal of Medicinal Chemistry (**1971**), 14(9), 827-33
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 15 (Pharmacodynamics)
OS CASREACT 75:128415
GI For diagram(s), see printed CA Issue.
AB When tested on mice with mammary tumors, 17β-bis(2-chloroethyl)aminoandrost-4-ene-3-one and 3-chloro-17β-bis(2-hydroxyethyl)aminoandrost-3,5-diene was ineffective and 17β-bis(2-chloroethyl)amino-5α-androst-2-ene (I) showed moderate antitumor activity. Synthetic studies and review of the literature showed that approaches involving N(CH2CH2OH)2 derivs. were the most reliable routes to steroidal N mustards where bonding of the mustard via a CN bond was required. The final chlorination step was critical When functional groups other than N(CH2CH2OH)2 were absent, POCl3 was the preferred chlorinating agent. When ketone or α,β-unsatd.

ketone functions were present, MeSO2Cl in pyridine was the reagent of choice. Mustard precursors containing primary or secondary OH functions may undergo chlorination with inversion using SOCl2. A review is given on the evaluation of the potential of steroid nitrogen mustards.

ST antitumor steroid nitrogen mustards; androstane nitrogen mustards

IT Mammary glands
(neoplasms of, steroidal nitrogen mustards effect on)

IT Neoplasm inhibitors
(steroidal nitrogen mustards)

IT Neoplasms
(steroidal nitrogen mustards effect on mammary)

IT Androsta-3,5-diene-17β-amine, 3-chloro-N,N-bis(2-hydroxyethyl)-
Ethanol, 2,2'-[(3-chloroandrosta-3,5-diene-17β-yl)imino]di-
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mammary neoplasm response to)

IT 33068-77-8 33068-79-0 34327-34-9 34327-35-0 34327-36-1
34327-38-3 34327-43-0 34327-44-1 34327-45-2 34327-46-3
34327-47-4 34336-34-0 34336-35-1
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)
(mammary neoplasm response to)

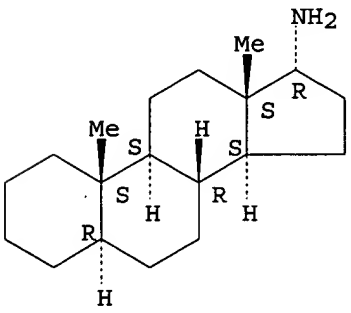
IT 1259-41-2P 1865-60-7P 3932-07-8P 31239-22-2P **31239-23-3P**
34327-37-2P 34327-39-4P 34327-42-9P 34327-48-5P 34336-31-7P
34336-32-8P 34336-33-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **31239-23-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 31239-23-3 HCAPLUS

CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 9 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1971:125901 HCAPLUS

DN 74:125901

ED Entered STN: 12 May 1984

TI Steroid alkaloids. CXIX. NMR spectrum of epimeric aminated steroids in the presence of Eu(dpm)3

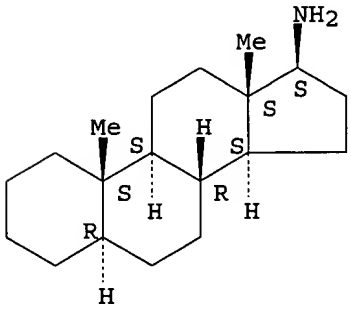
AU Lacombe, Liliane; Khuong-Huu-Laine, Francoise; Pancrazi, Ange; Khuong-Huu-Qui; Lukacs, Gabor

CS Lab. Chim. Org. Hormones, Coll. France, Paris, Fr.

SO Comptes Rendus des Seances de l'Academie des Sciences, Serie C: Sciences Chimiques (**1971**), 272(7), 668-71

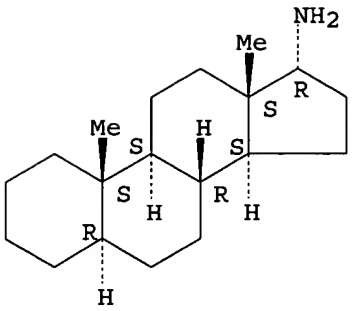
CODEN: CHDCAQ; ISSN: 0567-6541
DT Journal
LA French
CC 32 (Steroids)
AB By studying displacement of PMR chemical shifts in the presence of Eu(dpm)3 (dpm = dipivalomethanato) individual proton signals were assigned and the stereochemistry of the A/B and C/D ring junctions were determined in the epimeric amino steroids, 3α- and 3β-amino-5α-pregnane, and 17α- and 17β-amino-5α-androstane. As in complexes of other compds. with Eu(dpm)3, the signals of protons closest to Eu are displaced most.
ST steroids amino epimer NMR; europium dipivalomethanato aminosteroids NMR
IT Steroids, properties
RL: PRP (Properties)
(amino, N.M.R. of, in presence of europium complexes)
IT 15522-71-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(nuclear magnetic resonance of amino steroids in presence of)
IT 10308-45-9 10308-46-0 **31239-17-5 31239-23-3**
RL: PRP (Properties)
(nuclear magnetic resonance of, in presence of europium complex)
IT 1118-71-4DP, 3,5-Heptanedione, 2,2,6,6-tetramethyl-, europium complexes
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **31239-17-5 31239-23-3**
RL: PRP (Properties)
(nuclear magnetic resonance of, in presence of europium complex)
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



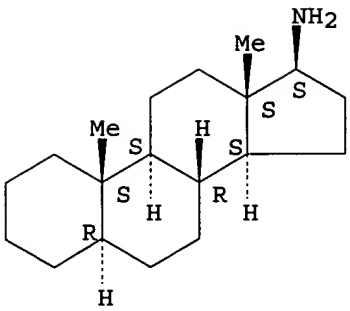
RN 31239-23-3 HCAPLUS
CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



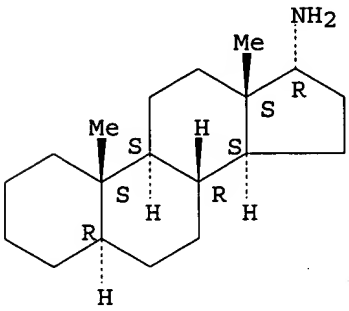
L34 ANSWER 10 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1971:88205 HCAPLUS
DN 74:88205
ED Entered STN: 12 May 1984
TI Steroid alkaloids. CVII. Photochemistry of azido steroids
AU Pancrazi, Ange; Khuong-Huu-Qui; Goutarel, Robert
CS Inst. Chim. Subst. Natur., CNRS, Gif-sur-Yvette, Fr.
SO Bulletin de la Societe Chimique de France (**1970**), (12), 4446-51
CODEN: BSCFAS; ISSN: 0037-8968
DT Journal
LA French
CC 32 (Steroids)
GI For diagram(s), see printed CA Issue.
AB Photolysis of nonaromatic azides occurs by formation of activated nitrenes which, in the presence of triplet quencher, isomerize to imines, and in the presence of a sensitizer, isomerize to imines or abstract H from the solvent to give primary amines. The photolysis of 3β,20α-diazidopregn-5-ene in cyclohexane failed to yield conessine (Barton, D. H. R. and Morgan, L. R., Jr., 1962). Reduction of the products with LiAlH4 gave mainly 3ξ,20ξ-bis(dimethylamino)-pregn-5-ene. The photolysis of 20α-azido-5α-pregnane yielded mainly the Schiff base (I), probably through dimerization of nitrenes followed by isomerization, elimination of 1 of the 2 N atoms, formation of radicals, and coupling.
ST photolysis azido pregnanes; azido pregnanes photolysis; pregnanes azido photolysis; irradn azomethines pregnanes; azomethines pregnanes irradn; conessines azido pregnanes
IT Steroids, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(azido, photolysis of)
IT 7332-00-5 31239-22-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(photolysis of)
IT 166-37-0DP, Cyclobuta[2,3]cyclopenta[1,2-a]phenanthrene, steroid derivs.
848-62-4P 963-74-6P 7707-71-3P 17291-32-6P 20853-63-8P
20853-64-9P 25829-97-4P **31239-17-5P 31239-23-3P**
31239-24-4P 31239-25-5P 31239-26-6P 31239-27-7P 31239-28-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **31239-17-5P 31239-23-3P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 31239-17-5 HCAPLUS
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 31239-23-3 HCAPLUS
CN Androstan-17-amine, (5α,17α)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L34 ANSWER 11 OF 11 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:76285 HCAPLUS
DN 66:76285
ED Entered STN: 12 May 1984
TI Synthesis of 3β-acetoxy-17β-(L-arginyl-L-arginyl-L-prolyl) amino-5 α-androstane
AU **Pettit, George R.**; Smith, Robert Lawrence; Klinger, J.
CS Univ. of Maine, Orono, ME, USA
SO Journal of Medicinal Chemistry (**1967**), 10(2), 145-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
GI For diagram(s), see printed CA Issue.
AB A steroidal peptide based on the 17-19 unit sequence of β-corticotropin was synthesized. Construction of the title substance (I) was achieved starting from 3β-hydroxy-17β-amino-5α-androstane. The phenylisoxazolium method was used for peptide bond formation and a combination of acetyl (for the steroid nucleus), carbobenzoxy, and nitro (for arginine) protecting groups were employed. I was characterized as the triacetate derivative and the assigned structure received addnl. support from results of an amino acid analysis.
ST CORTICOTROPINS STEROID PEPTIDES HORMONES; TRIPEPTIDES ANDROSTANES; STEROID PEPTIDES HORMONES CORTICOTROPINS; HORMONES CORTICOTROPINS STEROID PEPTIDES; ANDROSTANES TRIPEPTIDES; PEPTIDES STEROID HORMONES CORTICOTROPINS
IT 5α-Androstan-3β-ol, 17β-[1-[N2-[N2-carboxy-N5-

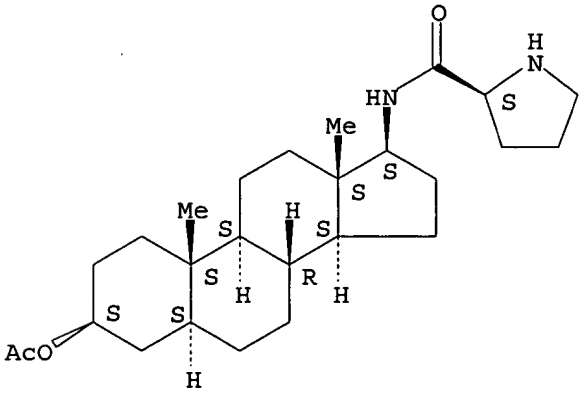
(nitroamidino)-L-ornithyl]-N5-(nitroamidino)-L-ornithyl]-2-pyrrolidinecarboxamido, benzyl ester, acetate (ester)
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate (ester), L-
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate ester, L-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 2149-70-4P 2304-98-5P 10463-56-6P 10463-58-8P 10463-59-9P
10463-60-2P 13574-67-9P **13574-69-1P 13574-72-6P**
13794-76-8P 13794-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **13574-69-1P 13574-72-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

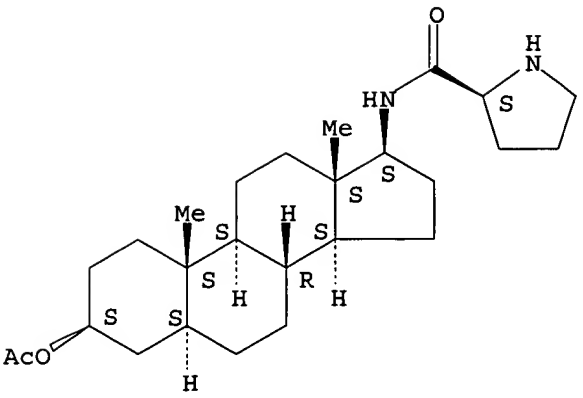
RN 13574-69-1 HCAPLUS
CN 2-Pyrrolidinecarboxamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 13574-72-6 HCAPLUS
CN 2-Pyrrolidinecarboxamide, N-(3β-hydroxy-5α-androstan-17β-yl)-, acetate (ester), monohydrochloride, L- (8CI) (CA INDEX NAME)

Absolute stereochemistry.



● HCl

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FILE 'USPATFULL' ENTERED AT 08:10:46 ON 24 AUG 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 23 Aug 2005 (20050823/PD)
FILE LAST UPDATED: 23 Aug 2005 (20050823/ED)
HIGHEST GRANTED PATENT NUMBER: US6934966
HIGHEST APPLICATION PUBLICATION NUMBER: US2005183181
CA INDEXING IS CURRENT THROUGH 23 Aug 2005 (20050823/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 23 Aug 2005 (20050823/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005
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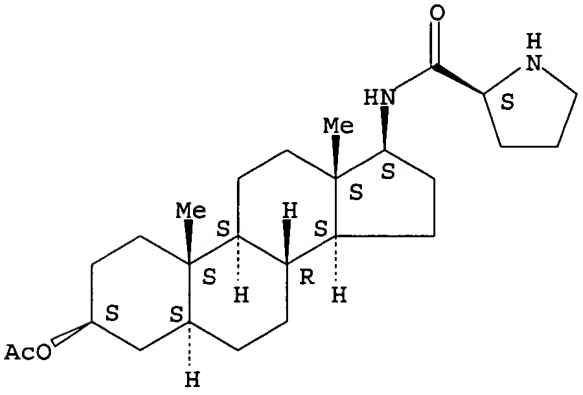
This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> d l35 bib abs hitstr tot

L35 ANSWER 1 OF 9 USPATFULL on STN
AN 2003:306925 USPATFULL
TI Therapeutic compositions effective against gram positive bacteria
IN Pettit, George R., Paradise Valley, AZ, UNITED STATES
Pettit, Robin K., Fountain Hills, AZ, UNITED STATES
PI US 2003216361 A1 20031120
AI US 2001-893861 A1 20010628 (9)
PRAI US 2000-214844P 20000628 (60)
DT Utility
FS APPLICATION
LREP FENNEMORE CRAIG, 3003 N. Central Avenue, Suite 2600, Phoenix, AZ, 85012
CLMN Number of Claims: 16
ECL Exemplary Claim: 1
DRWN 3 Drawing Page(s)
LN.CNT 755
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB The present invention relates to compounds of the formula ##STR1## and to pharmaceutically acceptable salts thereof, wherein R.sup.1 and R.sup.2 are as defined herein. The compounds are useful as anti-microbial agents, most specifically against gram positive bacteria. The invention further relates to pharmaceutical compositions and methods of treating bacterial infection using such compositions.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **13574-69-1**
(androstane amides effective against Gram-pos. bacteria)
RN 13574-69-1 USPATFULL
CN 2-Pyrrolidinecarboxamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

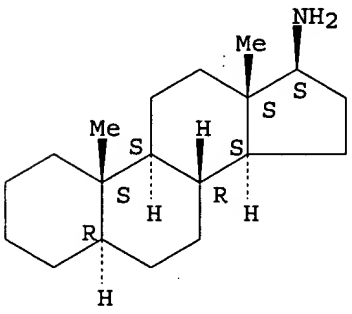


L35 ANSWER 2 OF 9 USPATFULL on STN
AN 97:31841 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Kalamazoo, MI, United States
Wallach, legal representative, Vera M., Richland, MI, United States
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)

PI US 5621123 19970415
AI US 1994-247169 19940520 (8)
DCD 20100216
RLI Division of Ser. No. US 1992-976751, filed on 16 Nov 1992, now patented, Pat. No. US 5334712, issued on 2 Aug 1994 which is a division of Ser. No. US 1991-657721, filed on 20 Feb 1991, now patented, Pat. No. US 5196542, issued on 23 Mar 1993 which is a division of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Shah, Mukund J.; Assistant Examiner: Sripada, Pavanaram K.
LREP Wootton, Thomas A.
CLMN Number of Claims: 4
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 368
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

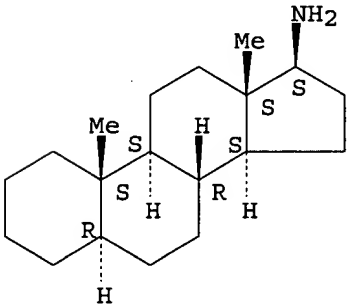


L35 ANSWER 3 OF 9 USPATFULL on STN
AN 94:109016 USPATFULL
TI Steroid compounds
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Richland, MI, United States by Vera M. Wallach, legal representative
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5373095 19941213

AI US 1993-126153 19930923 (8)
RLI Division of Ser. No. US 1992-972693, filed on 6 Nov 1992, now patented, Pat. No. US 5274089 which is a division of Ser. No. US 1991-793486, filed on 13 Nov 1991, now patented, Pat. No. US 5187299 which is a continuation of Ser. No. US 1991-657729, filed on 20 Feb 1991, now abandoned which is a division of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 8 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Richter, Johann; Assistant Examiner: Cook, Rebecca
LREP Wootton, Thomas A.
CLMN Number of Claims: 2
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4711
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



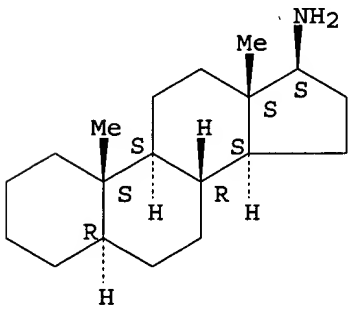
L35 ANSWER 4 OF 9 USPATFULL on STN
AN 94:66602 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Richland, MI, United States by Vera M. Wallach, Legal Representative
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5334712 19940802
AI US 1992-976751 19921116 (7)
RLI Division of Ser. No. US 1991-657721, filed on 20 Feb 1991, now patented,

Pat. No. US 5196524, issued on 23 Mar 1993 which is a division of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned

DT Utility
FS Granted
EXNAM Primary Examiner: Shahl, Mukund J.; Assistant Examiner: Sripada, P. K.
LREP Wootton, Thomas A.
CLMN Number of Claims: 5
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4587
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

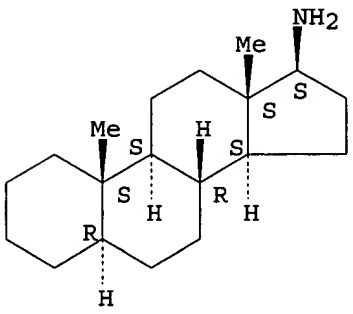


L35 ANSWER 5 OF 9 USPATFULL on STN
AN 93:109187 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Bundy, Gordon L., Kalamazoo, MI, United States
Wallach, deceased, Donald P., late of Richland, MI, United States by Vera M. Wallach, legal representative
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5274089 19931228
AI US 1992-972693 19921106 (7)
RLI Division of Ser. No. US 1991-793486, filed on 13 Nov 1991, now patented, Pat. No. US 5187299 which is a continuation of Ser. No. US 1991-657729, filed on 20 Feb 1991, now abandoned which is a division of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation of Ser. No. US 1986-102116, filed on 7 Oct 1986, now abandoned which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a

continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Cintins, Marianne M.; Assistant Examiner: Kestler, Kimberly J.
LREP Wootton, Thomas A.
CLMN Number of Claims: 3
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4555
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

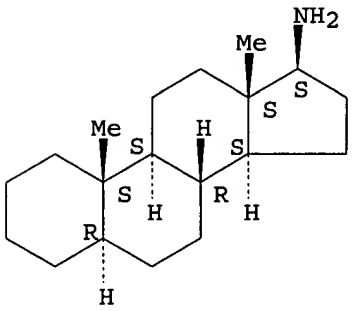


L35 ANSWER 6 OF 9 USPATFULL on STN
AN 93:22826 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Richland, MI, United States by Vera M. Wallach, legal representative
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5196542 19930323
AI US 1991-657721 19910220 (7)
RLI Division of Ser. No. US 1989-394396, filed on 15 Aug 1989 which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Bond, Robert T.

LREP Wright, Debbie K., Wootton, Thomas A.
CLMN Number of Claims: 3
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4544
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

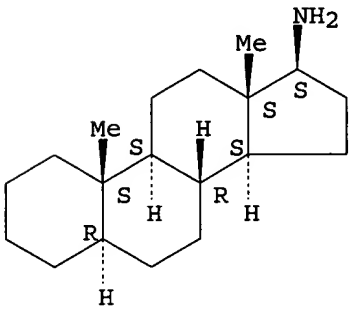


L35 ANSWER 7 OF 9 USPATFULL on STN
AN 93:12656 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Portage, MI, United States
Wallach, Legal Representative, by Vera M., Richland, MI, United States
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5187299 19930216
AI US 1991-793486 19911113 (7)
RLI Continuation of Ser. No. US 1991-657729, filed on 20 Feb 1991, now abandoned which is a division of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Cintins, Marianne M.; Assistant Examiner: Kestler, Kimberly J.
LREP Koivuniemi, Paul J., Wright, Debbie K., Wootton, Thomas A.
CLMN Number of Claims: 5
ECL Exemplary Claim: 1
DRWN No Drawings

LN.CNT 4473
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

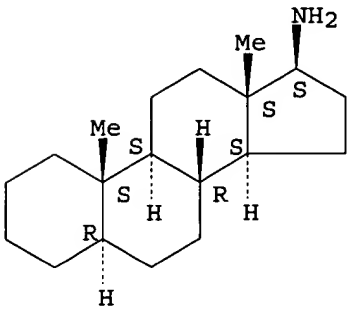


L35 ANSWER 8 OF 9 USPATFULL on STN
AN 92:74640 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Kalamazoo, MI, United States
Wallach, legal representative, by Vera M., Richland, MI, United States
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 5145874 19920908
AI US 1991-663037 19910225 (7)
RLI Continuation of Ser. No. US 1989-394396, filed on 15 Aug 1989, now abandoned which is a division of Ser. No. US 1987-117851, filed on 16 Jun 1987, now patented, Pat. No. US 4917826 which is a continuation-in-part of Ser. No. US 1986-843120, filed on 24 Mar 1986, now abandoned which is a continuation-in-part of Ser. No. US 1985-788995, filed on 18 Oct 1985, now abandoned
DT Utility
FS Granted
EXNAM Primary Examiner: Richter, Johann
LREP Wootton, Thomas A., Wright, Debbie K., Koivuniemi, Paul J.
CLMN Number of Claims: 8
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4780
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

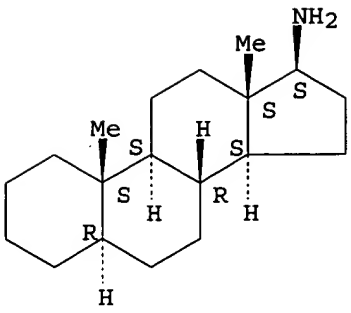
Absolute stereochemistry.



L35 ANSWER 9 OF 9 USPATFULL on STN
AN 90:29778 USPATFULL
TI Cyclic hydrocarbons with an aminoalkyl sidechain
IN Johnson, Roy A., Kalamazoo, MI, United States
Bundy, Gordon L., Portage, MI, United States
Youngdale, Gilbert A., Portage, MI, United States
Morton, Douglas R., Portage, MI, United States
Wallach, deceased, Donald P., late of Kalamazoo, MI, United States by Vera M. Wallach, legal representative
PA The Upjohn Company, Kalamazoo, MI, United States (U.S. corporation)
PI US 4917826 19900417
WO 8702367 19870423
AI US 1987-117851 19870616 (7)
WO 1986-US2116 19861007
19870616 PCT 371 date
19870616 PCT 102(e) date
DT Utility
FS Granted
EXNAM Primary Examiner: Lee, Mary C.; Assistant Examiner: Richter, J.
LREP Koivuniemi, Paul J.
CLMN Number of Claims: 3
ECL Exemplary Claim: 1
DRWN No Drawings
LN.CNT 4514
CAS INDEXING IS AVAILABLE FOR THIS PATENT.
AB Provided are cyclic hydrocarbons of Formula I ##STR1## with an aminoalkyl sidechain that are useful for treating phospholipase A2 mediated conditions, diabetes, and obesity.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.
IT **31239-17-5**, 5α-Androstan-17β-amine
(reaction of, in synthesis of phospholipase A2-inhibiting amino steroids and analogs)
RN 31239-17-5 USPATFULL
CN Androstan-17-amine, (5α,17β)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES:   22 AUG 2005  HIGHEST RN 861291-85-2
DICTIONARY FILE UPDATES:  22 AUG 2005  HIGHEST RN 861291-85-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

*************************************************************************
*                                                                       *
* The CA roles and document type information have been removed from     *
* the IDE default display format and the ED field has been added,       *
* effective March 20, 2005.  A new display format, IDERL, is now        *
* available and contains the CA role and document type information.     *
*                                                                       *
*************************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

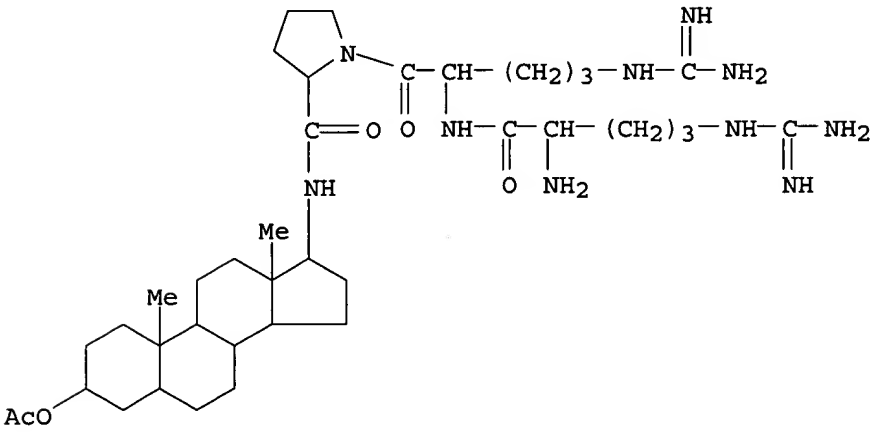
=> d ide can tot l54

L54  ANSWER 1 OF 6  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   13794-77-9  REGISTRY
ED   Entered STN:  16 Nov 1984
CN   2-Pyrrolidinecarboxamide, 1-(N2-L-arginyl-L-arginyl)-N-(3β-hydroxy-
     5α-androstan-17β-yl)-, acetate (ester), triacetate, L- (8CI)
     (CA INDEX NAME)
OTHER CA INDEX NAMES:
```

CN 5α-Androstan-3β-ol, 17β-[1-(N2-L-arginyl-L-arginyl)-L-2-pyrrolidinecarboxamido]-, acetate (ester), triacetate
MF **C38 H66 N10 O5 . 3 C2 H4 O2**
LC STN Files: CA, CAPLUS

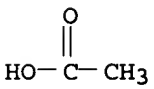
CM 1

CRN 10463-56-6
CMF C38 H66 N10 O5



CM 2

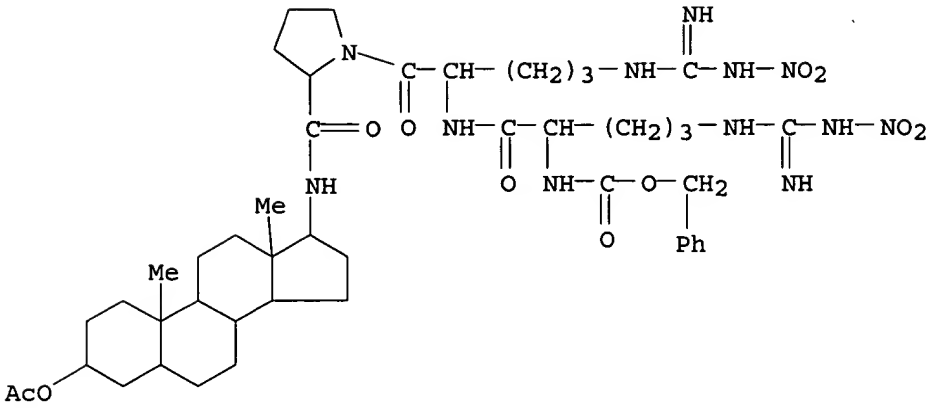
CRN 64-19-7
CMF C2 H4 O2



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

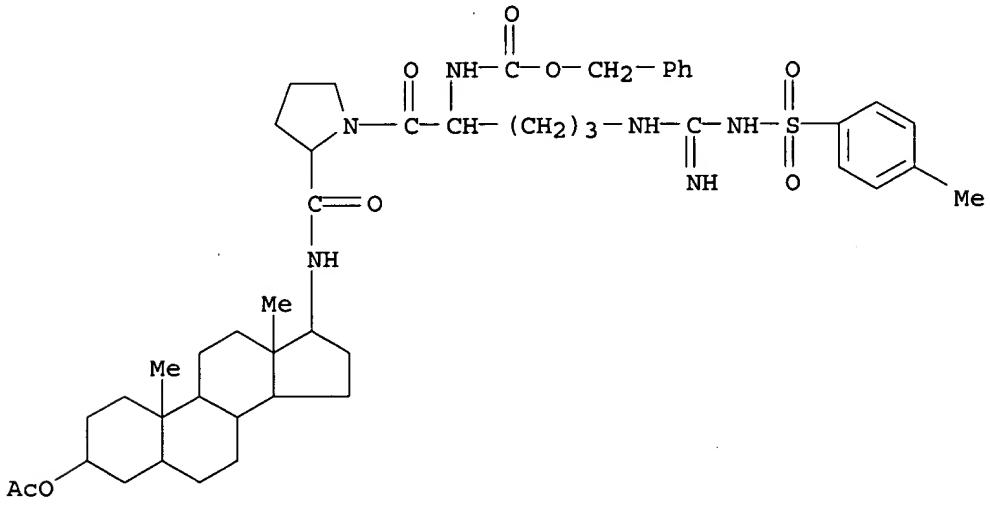
L54 ANSWER 2 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN **13794-76-8** REGISTRY
ED Entered STN: 16 Nov 1984
CN Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate (ester), L- (8CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5α-Androstan-3β-ol, 17β-[1-[N2-[N2-carboxy-N5-(nitroamidino)-L-ornithyl]-N5-(nitroamidino)-L-ornithyl]-N5-(nitroamidino)-L-ornithyl]-2-pyrrolidinecarboxamidino]-, benzyl ester, acetate (ester)
MF **C46 H70 N12 O11**
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

L54 ANSWER 3 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN **13650-37-8** REGISTRY
ED Entered STN: 16 Nov 1984
CN Carbamic acid, [1-[[2-[(3β-hydroxy-5α-androstan-17β-yl)carbamoyl]-1-pyrrolidinyl]carbonyl]-4-[3-(p-tolylsulfonyl)guanidino]butyl]-, benzyl ester, acetate (ester) (8CI) (CA INDEX NAME)
MF **C47 H66 N6 O8 S**
LC STN Files: CA, CAPLUS

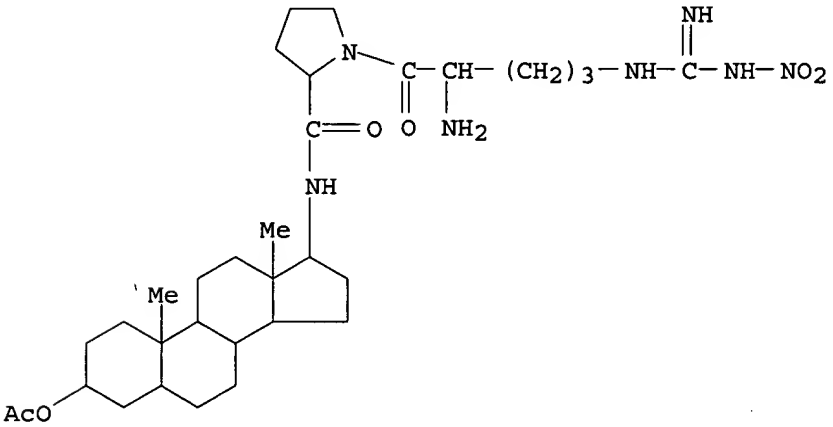


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:95380

L54 ANSWER 4 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN **10463-60-2** REGISTRY
ED Entered STN: 16 Nov 1984
CN L-Prolinamide, N5-[imino(nitroamino)methyl]-L-ornithyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, monohydrochloride (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pyrrolidinecarboxamide, N-(3β-hydroxy-5α-androstan-17β-yl)-1-[N5-(nitroamidino)-L-ornithyl]-, acetate (ester), monohydrochloride, L- (8CI)
CN Androstane, L-prolinamide deriv.
MF **C32 H53 N7 O6 . Cl H**
LC STN Files: CA, CAPLUS
CRN (10463-89-5)



● HCl

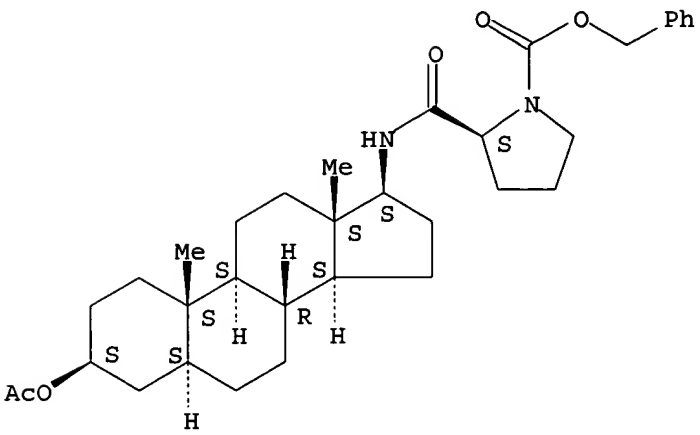
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

L54 ANSWER 5 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN **10463-58-8** REGISTRY
ED Entered STN: 16 Nov 1984
CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]amino]carbonyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 1-Pyrrolidinecarboxylic acid, 2-[(3β-hydroxy-5α-androstan-17β-yl)carbamoyl]-, benzyl ester, acetate (ester), L- (8CI)
CN 5α-Androstan-3β-ol, 17β-(1-carboxy-L-2-pyrrolidinecarboxamido)-, benzyl ester, acetate (ester)
CN Androstane, 1-pyrrolidinecarboxylic acid deriv.
FS STEREOSEARCH
MF **C34 H48 N2 O5**
LC STN Files: BEILSTEIN*, CA, CAPLUS

(*File contains numerically searchable property data)

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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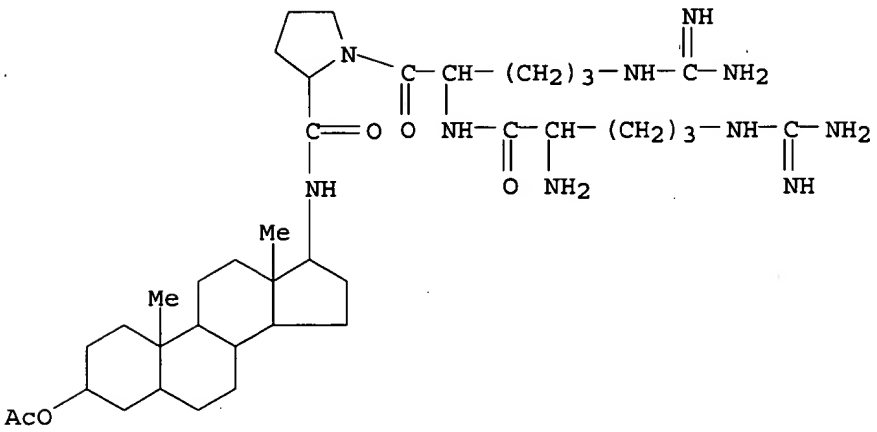
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

L54 ANSWER 6 OF 6 REGISTRY COPYRIGHT 2005 ACS on STN
RN **10463-56-6** REGISTRY
ED Entered STN: 16 Nov 1984
CN L-Prolinamide, L-arginyl-L-arginyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Pyrrolidinecarboxamide, 1-(N2-L-arginyl-L-arginyl)-N-(3β-hydroxy-5α-androstan-17β-yl)-, acetate (ester), L- (8CI)
CN 5α-Androstan-3β-ol, 17β-[1-(N2-L-arginyl-L-arginyl)-L-2-pyrrolidinecarboxamido]-, acetate (ester)
CN Androstane, L-prolinamide deriv.
MF **C38 H66 N10 O5**
CI COM
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

=> d his l54-

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FILE 'REGISTRY' ENTERED AT 08:18:36 ON 24 AUG 2005
L54 6 S L40 NOT C53H75N9O9S2

FILE 'HCAOLD' ENTERED AT 08:19:05 ON 24 AUG 2005
L55 0 S L54

FILE 'HCAPLUS' ENTERED AT 08:19:08 ON 24 AUG 2005
L56 2 S L54
L57 2 S L56 AND L1-L5

FILE 'USPATFULL' ENTERED AT 08:19:28 ON 24 AUG 2005
L58 0 S L54

FILE 'REGISTRY' ENTERED AT 08:19:42 ON 24 AUG 2005

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:19:57 ON 24 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

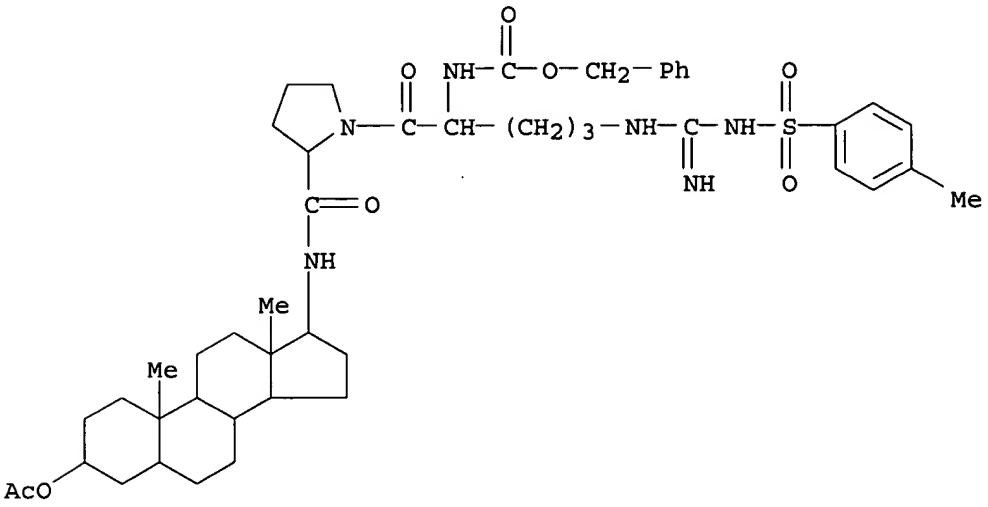
FILE COVERS 1907 - 24 Aug 2005 VOL 143 ISS 9
FILE LAST UPDATED: 23 Aug 2005 (20050823/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l57 all hitstr tot

L57 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:95380 HCAPLUS
DN 66:95380
ED Entered STN: 12 May 1984
TI Steroids and related natural products. XXXVII. Structural biochemistry. 5. Diarginyl steroidal peptides
AU **Pettit, George R.**; Das Gupta, Arun K.
CS Univ. of Maine, Orono, ME, USA
SO Canadian Journal of Chemistry (1967), 45(5), 567-70
CODEN: CJCHAG; ISSN: 0008-4042
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
GI For diagram(s), see printed CA Issue.
AB cf. preceding abstract 5α-Androstanes (I) and 3β-hydroxyandrost-5-enes (II), where X is OH or OAc and Y is a N-(polypeptide residue)amino group, are prepared
IT Steroids, preparation
RL: PREP (Preparation)
(peptide derivs.)
IT Peptides, preparation
RL: PREP (Preparation)
(steroidal)
IT 74-79-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(peptides containing, steroidal)
IT 3249-05-6P 3249-07-8P 13650-29-8P 13650-30-1P 13650-32-3P 13650-33-4P 13650-34-5P 13650-36-7P **13650-37-8P** 13650-38-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **13650-37-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 13650-37-8 HCAPLUS
CN Carbamic acid, [1-[[2-[(3β-hydroxy-5α-androstan-17β-yl)carbamoyl]-1-pyrrolidinyl]carbonyl]-4-[3-(p-tolylsulfonyl)guanidino]butyl]-, benzyl ester, acetate (ester) (8CI) (CA INDEX NAME)

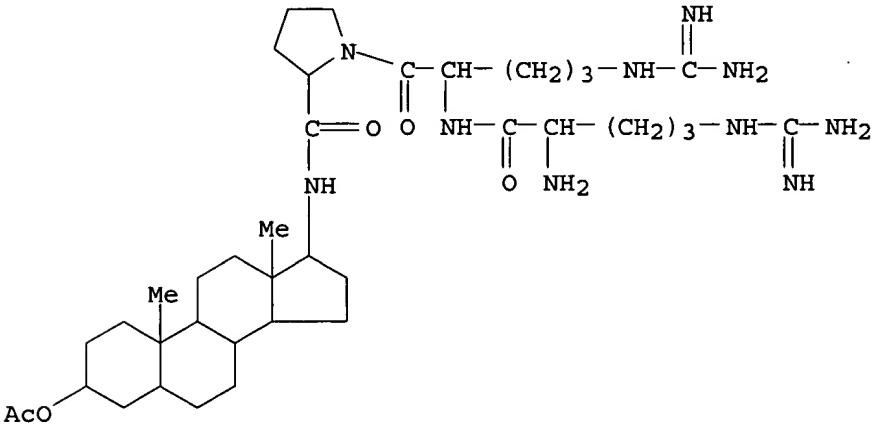


L57 ANSWER 2 OF 2 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:76285 HCAPLUS
DN 66:76285
ED Entered STN: 12 May 1984
TI Synthesis of 3β-acetoxy-17β-(L-arginyl-L-arginyl-L-prolyl) amino-5 α-androstane
AU **Pettit, George R.**; Smith, Robert Lawrence; Klinger, J.
CS Univ. of Maine, Orono, ME, USA
SO Journal of Medicinal Chemistry (1967), 10(2), 145-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
GI For diagram(s), see printed CA Issue.
AB A steroidal peptide based on the 17-19 unit sequence of β-corticotropin was synthesized. Construction of the title substance (I) was achieved starting from 3β-hydroxy-17β-amino-5α-androstane. The phenylisoxazolium method was used for peptide bond formation and a combination of acetyl (for the steroid nucleus), carbobenzoxy, and nitro (for arginine) protecting groups were employed. I was characterized as the triacetate derivative and the assigned structure received addnl. support from results of an amino acid analysis.
ST CORTICOTROPINS STEROID PEPTIDES HORMONES; TRIPEPTIDES ANDROSTANES; STEROID PEPTIDES HORMONES CORTICOTROPINS; HORMONES CORTICOTROPINS STEROID PEPTIDES; ANDROSTANES TRIPEPTIDES; PEPTIDES STEROID HORMONES CORTICOTROPINS
IT 5α-Androstan-3β-ol, 17β-[1-[N2-[N2-carboxy-N5-(nitroamidino)-L-ornithyl]-N5-(nitroamidino)-L-ornithyl]-2-pyrrolidinecarboxamido, benzyl ester, acetate (ester)
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate (ester), L-
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate ester, L-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 2149-70-4P 2304-98-5P **10463-56-6P 10463-58-8P**

10463-59-9P **10463-60-2P** 13574-67-9P 13574-69-1P
13574-72-6P **13794-76-8P 13794-77-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

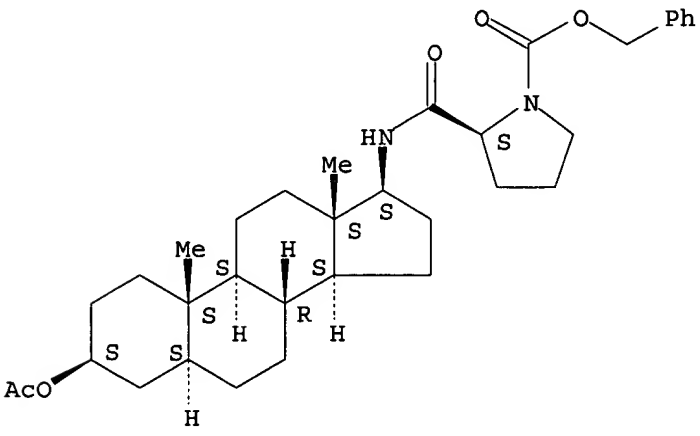
IT **10463-56-6P 10463-58-8P 10463-60-2P**
13794-76-8P 13794-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 10463-56-6 HCAPLUS
CN L-Prolinamide, L-arginyl-L-arginyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]- (9CI) (CA INDEX NAME)

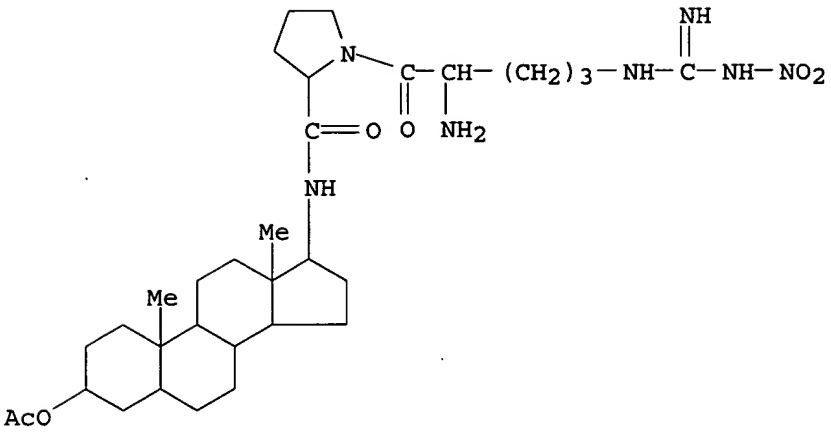


RN 10463-58-8 HCAPLUS
CN 1-Pyrrolidinecarboxylic acid, 2-[[[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]amino]carbonyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

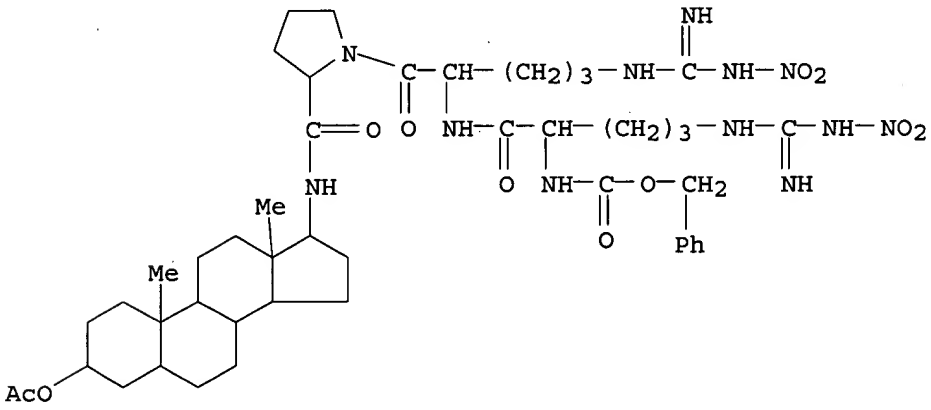


RN 10463-60-2 HCAPLUS
CN L-Prolinamide, N5-[imino(nitroamino)methyl]-L-ornithyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

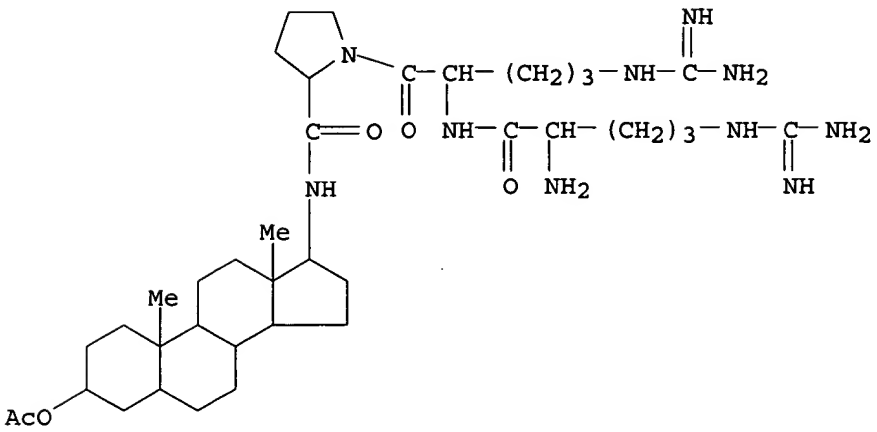
RN 13794-76-8 HCAPLUS
CN Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate (ester), L- (8CI) (CA INDEX NAME)



RN 13794-77-9 HCAPLUS
CN 2-Pyrrolidinecarboxamide, 1-(N2-L-arginyl-L-arginyl)-N-(3β-hydroxy-5α-androstan-17β-yl)-, acetate (ester), triacetate, L- (8CI) (CA INDEX NAME)

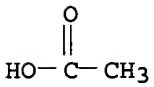
CM 1

CRN 10463-56-6
CMF C38 H66 N10 O5



CM 2

CRN 64-19-7
CMF C2 H4 O2



=> => fil reg
FILE 'REGISTRY' ENTERED AT 08:30:34 ON 24 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES: 22 AUG 2005 HIGHEST RN 861291-85-2
DICTIONARY FILE UPDATES: 22 AUG 2005 HIGHEST RN 861291-85-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

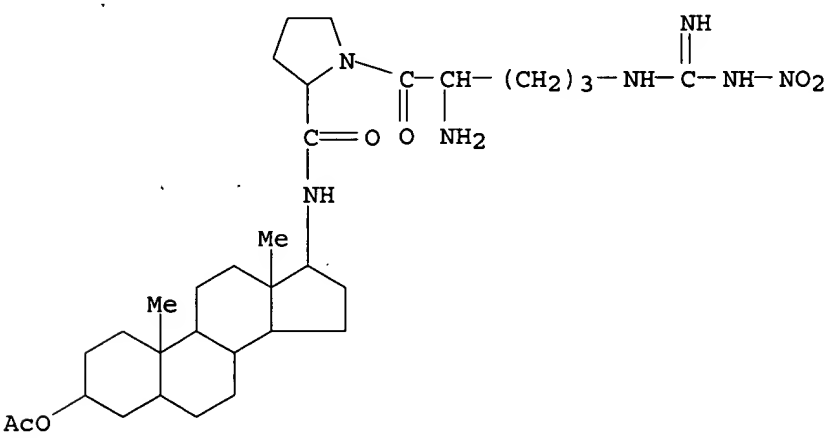
```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

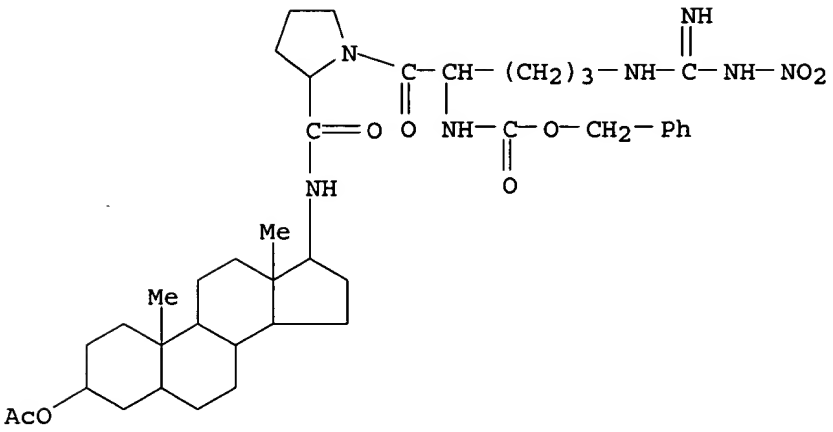
=> d l68 ide can tot

L68 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
RN 10463-89-5 REGISTRY
ED Entered STN: 16 Nov 1984
CN L-Prolinamide, N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-1-[N5-[imino(nitroamino)methyl]-L-ornithyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Androstane, L-prolinamide deriv.
MF **C32 H53 N7 O6**
CI COM



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

L68 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
RN 10463-59-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN L-Prolinamide, N5-[imino(nitroamino)methyl]-N2-[(phenylmethoxy)carbonyl]-L-ornithyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5α-Androstan-3β-ol, 17β-[1-[N2-carboxy-N5-(nitroamidino)-L-ornithyl]-L-2-pyrrolidinecarboxamido]-, benzyl ester, acetate (ester)
CN Androstane, L-prolinamide deriv.
CN Carbamic acid, [1-[[2-[(3β-hydroxy-5α-androstan-17β-yl)carbamoyl]-1-pyrrolidinyl]carbonyl]-4-(3-nitroguanidino)butyl]-, benzyl ester, acetate (ester) (8CI)
MF **C40 H59 N7 O8**
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 66:76285

=> fil hcaplus
FILE 'HCAPLUS' ENTERED AT 08:30:39 ON 24 AUG 2005
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 24 Aug 2005 VOL 143 ISS 9
FILE LAST UPDATED: 23 Aug 2005 (20050823/ED)

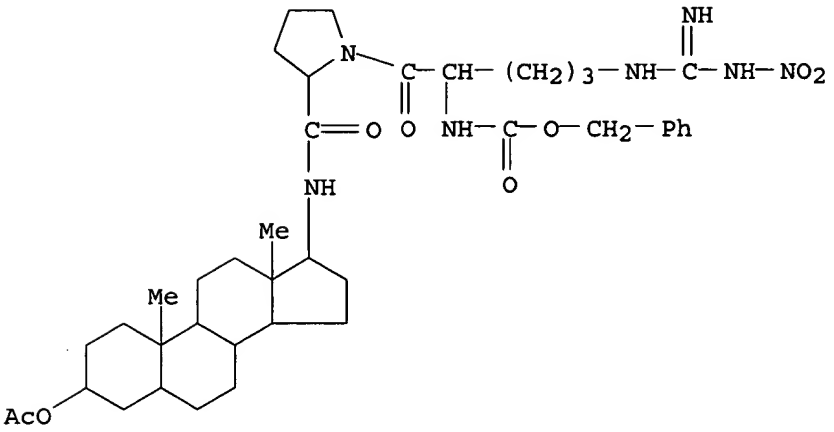
New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d all hitstr l71

L71 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN
AN 1967:76285 HCAPLUS
DN 66:76285
ED Entered STN: 12 May 1984
TI Synthesis of 3β-acetoxy-17β-(L-arginyl-L-arginyl-L-prolyl) amino-5 α-androstane

AU **Pettit, George R.**; Smith, Robert Lawrence; Klinger, J.
CS Univ. of Maine, Orono, ME, USA
SO Journal of Medicinal Chemistry (1967), 10(2), 145-8
CODEN: JMCMAR; ISSN: 0022-2623
DT Journal
LA English
CC 34 (Synthesis of Amino Acids, Peptides, and Proteins)
GI For diagram(s), see printed CA Issue.
AB A steroidal peptide based on the 17-19 unit sequence of β-corticotropin was synthesized. Construction of the title substance (I) was achieved starting from 3β-hydroxy-17β-amino-5α-androstane. The phenylisoxazolium method was used for peptide bond formation and a combination of acetyl (for the steroid nucleus), carbobenzoxy, and nitro (for arginine) protecting groups were employed. I was characterized as the triacetate derivative and the assigned structure received addnl. support from results of an amino acid analysis.
ST CORTICOTROPINS STEROID PEPTIDES HORMONES; TRIPEPTIDES ANDROSTANES; STEROID PEPTIDES HORMONES CORTICOTROPINS; HORMONES CORTICOTROPINS STEROID PEPTIDES; ANDROSTANES TRIPEPTIDES; PEPTIDES STEROID HORMONES CORTICOTROPINS
IT 5α-Androstan-3β-ol, 17β-[1-[N2-[N2-carboxy-N5-(nitroamidino)-L-ornithyl]-N5-(nitroamidino)-L-ornithyl]-2-pyrrolidinecarboxamido, benzyl ester, acetate (ester)
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate (ester), L-
Prolinamide, Nα-carboxy-NG-nitro-L-arginyl-NG-nitro-L-arginyl-N-(3β-hydroxy-5α-androstan-17β-yl)-, benzyl ester, acetate ester, L-
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT 2149-70-4P 2304-98-5P 10463-56-6P 10463-58-8P **10463-59-9P**
10463-60-2P 13574-67-9P 13574-69-1P 13574-72-6P 13794-76-8P
13794-77-9P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
IT **10463-59-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 10463-59-9 HCAPLUS
CN L-Prolinamide, N5-[imino(nitroamino)methyl]-N2-[(phenylmethoxy)carbonyl]-L-ornithyl-N-[(3β,5α,17β)-3-(acetyloxy)androstan-17-yl]-
(9CI) (CA INDEX NAME)



=> => d his

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L1            1 S US20030216361/PN OR (US2001-893861# OR US2000-214844#)/AP,PRN
                E PETTIT G/AU
L2           73 S E3,E9,E10
L3          696 S E14-E16,E21-E24
L4            1 S E26
L5          162 S E112,E118,E135,E136
                SEL RN L1

     FILE 'REGISTRY' ENTERED AT 07:48:03 ON 24 AUG 2005
L6            5 S E1-E5
L7            1 S L6 AND C5-C6-C6-C6/ES AND N/ELS
                E C26H42N2O3/MF
L8            1 S E3 AND C5-C6-C6-C6/ES AND NC4/ES
L9            1 S 13574-69-1/CRN
L10           2 S L7-L9
                E 4432.3/RID
L11       83023 S E4
L12       29539 S L11 AND N/ELS
L13           STR
L14          30 S L13 CSS
L15         758 S L13 CSS FUL
                SAV L15 KANTAM893/A
L16           STR L13
L17           0 S L16 CSS SAM SUB=L15
L18           0 S L15 AND SQL/FA
L19           STR L16
L20           2 S L19 CSS SAM SUB=L15
L21          93 S L19 CSS FUL SUB=L15
                SAV L21 KANTAM893A/A
L22           7 S L21 AND C19H33N
L23           9 S L10,L22
                SAV L23 KANTAM893B/A

     FILE 'HCAOLD' ENTERED AT 08:03:20 ON 24 AUG 2005
L24           2 S L23
                SEL AN
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                EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 08:04:21 ON 24 AUG 2005
L25             4 S E1-E2
L26             2 S L25 NOT (METHYLESTRADIOL OR ERGOSTEROL)/TI
L27            13 S L23
L28             2 S L26 AND L27
L29            11 S L27 NOT L28
L30             3 S L29 AND L1-L5
L31            12 S L27 AND (PD<=20000628 OR PRD<=20000628 OR AD<=20000628)
L32            11 S L26-L31 NOT L28
L33             2 S (3 BETA OR 3BETA OR 3B OR E B)()ACETOXY()(17BETA OR 17B OR 17
L34            11 S L32,L33

     FILE 'USPATFULL' ENTERED AT 08:08:28 ON 24 AUG 2005
L35             9 S L23

     FILE 'REGISTRY' ENTERED AT 08:08:57 ON 24 AUG 2005

     FILE 'HCAOLD' ENTERED AT 08:09:14 ON 24 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 08:09:29 ON 24 AUG 2005

     FILE 'USPATFULL' ENTERED AT 08:10:46 ON 24 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 08:11:17 ON 24 AUG 2005
L36             5 S L15 AND L2-L5
                SEL RN

     FILE 'REGISTRY' ENTERED AT 08:11:55 ON 24 AUG 2005
L37            36 S E3-E38
L38            20 S L37 AND L15
L39            18 S L38 NOT L23
L40             7 S L39 AND (C32H53N7O6 OR C38H66N10O5 OR C34H48N2O5 OR C47H66N6O
L41            16 S L37 NOT L38

     FILE 'HCAOLD' ENTERED AT 08:15:33 ON 24 AUG 2005
L42             1 S L40
                SEL AN
                EDIT /AN /OREF

     FILE 'HCAPLUS' ENTERED AT 08:15:50 ON 24 AUG 2005
L43             2 S E39
L44             1 S L43 NOT HALPERN?/AU
L45             3 S L40
L46             2 S L45 AND L1-L5
L47             4 S L44-L46
L48             3 S L47 NOT L44
L49             3 S L44-L48 AND PETTIT ?/AU
L50             2 S L45 AND L49
L51             3 S L45,L50
L52             1 S L49 NOT L51

     FILE 'USPATFULL' ENTERED AT 08:17:23 ON 24 AUG 2005
L53             0 S L40

     FILE 'REGISTRY' ENTERED AT 08:17:31 ON 24 AUG 2005

     FILE 'HCAOLD' ENTERED AT 08:17:40 ON 24 AUG 2005
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     FILE 'REGISTRY' ENTERED AT 08:18:36 ON 24 AUG 2005
L54           6 S L40 NOT C53H75N9O9S2

     FILE 'HCAOLD' ENTERED AT 08:19:05 ON 24 AUG 2005
L55           0 S L54

     FILE 'HCAPLUS' ENTERED AT 08:19:08 ON 24 AUG 2005
L56           2 S L54
L57           2 S L56 AND L1-L5

     FILE 'USPATFULL' ENTERED AT 08:19:28 ON 24 AUG 2005
L58           0 S L54

     FILE 'REGISTRY' ENTERED AT 08:19:42 ON 24 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 08:19:57 ON 24 AUG 2005

     FILE 'REGISTRY' ENTERED AT 08:20:10 ON 24 AUG 2005
L59             STR L19
L60           0 S L59 CSS SAM SUB=L15
L61          59 S L59 CSS FUL SUB=L15
               SAV L61 KANTAM893C/A
L62           0 S L61 NOT L21,L54
L63             STR
L64           1 S L63 SAM SUB=L15
L65          49 S L63 FUL SUB=L15
               SAV L65 KANTAM893D/A
L66          42 S L65 NOT L21,L54,L61
L67           4 S L66 AND (C26H42N2O3 OR C40H59N7O8 OR C32H53N7O6)
L68           2 S L67 NOT L23,L54

     FILE 'HCAOLD' ENTERED AT 08:29:43 ON 24 AUG 2005
L69           0 S L68

     FILE 'HCAPLUS' ENTERED AT 08:29:47 ON 24 AUG 2005
L70           1 S L68
L71           1 S L70 AND L1-L5

     FILE 'USPATFULL' ENTERED AT 08:30:11 ON 24 AUG 2005
L72           0 S L68

     FILE 'REGISTRY' ENTERED AT 08:30:34 ON 24 AUG 2005

     FILE 'HCAPLUS' ENTERED AT 08:30:39 ON 24 AUG 2005

=> => d que l65
L13             STR
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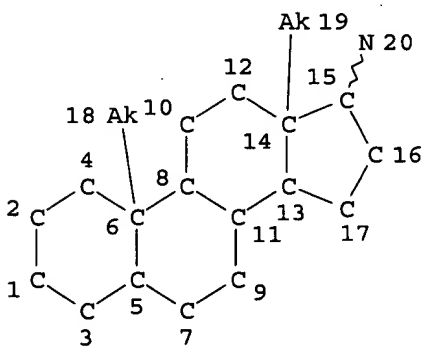

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CONNECT IS M1  RC AT   1
CONNECT IS M1  RC AT  20
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC   1
NUMBER OF NODES IS  20

STEREO ATTRIBUTES: NONE
L15          758 SEA FILE=REGISTRY CSS FUL L13
L63              STR
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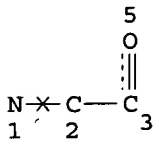


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NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS   4

STEREO ATTRIBUTES: NONE
L65           49 SEA FILE=REGISTRY SUB=L15 SSS FUL L63


=>
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